

THERMO-CHEMICAL MODELLING OF TWO-STAGE SMELTING REDUCTION PROCESS FOR IRONMAKING

by
LOKESH PANDEY

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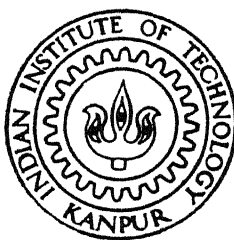
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DEPARTMENT OF MATERIALS AND METALLURGICAL ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

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THERMO-CHEMICAL MODELLING OF TWO-STAGE SMELTING REDUCTION PROCESS FOR IRONMAKING

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By

LOKESH PANDEY

To the

**DEPARTMENT OF MATERIALS
&
METALLURGICAL ENGINEERING**

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January 1997

Dedicated to my parents

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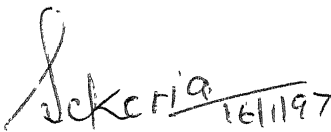
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CERTIFICATE

This is to certify that the work contained in the thesis entitled 'THERMO-CHEMICAL MODELLING OF TWO-STAGE SMELTING REDUCTION PROCESS FOR IRONMAKING' by LOKESH PANDEY has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

January, 1997


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LIST OF SYMBOLS

(All expressed in per kg mole of product Fe)

$n_{Fe}^i, n_C^i, n_{Si}^i, n_{Mn}^i, n_S^i, n_P^i, n_O^i, n_H^i, n_N^i, n_{Ca}^i, n_{Al_2O_3}^i$	kg moles of respective element or oxide in
$n_{Fe}^o, n_C^o, n_{Si}^o, n_{Mn}^o, n_S^o, n_P^o, n_O^o, n_H^o, n_N^o, n_{Ca}^o, n_{Al_2O_3}^o$	kg moles of respective element or oxide out
$n_C^{coal}, n_{SiO_2}^{coal}, n_S^{coal}, n_{Al_2O_3}^{coal}$	kg moles of respective element or oxide in coal
$n_{SiO_2}^{ore}, n_{Al_2O_3}^{ore}, n_{FeS}^{ore}, n_{SiO_2}^{ore}, n_{P_2O_5}^{ore}, n_{MnO}^{ore}$	kg moles of respective compound in ore
$C/Fe, Si/Fe, Mn/Fe, S/Fe, P/Fe$	kg moles of respective element in hot metal
$n_{CaO}, n_{SiO_2}, n_{MnO}, n_{MgO}, n_{Al_2O_3}, n_{CaS}$	kg moles of respective compound in slag
n_{CaCO_3}	kg moles of $CaCO_3$
n_{Fe}	kg moles of Fe leaving reduction shaft furnace
$n_{Fe_{0.95}O}$	kg moles of $Fe_{0.95}O$ leaving reduction shaft furnace
C_X	kg coal
Q_{MG}	Melter-gasifier heat losses (KJ)
Q_{RS}	Reduction shaft furnace heat losses (KJ)
D_{MG}	Melter gasifier heat demand (KJ)
D_{RS}	Reduction shaft furnace heat demand (KJ)

d_{rg}	Sensible heat loss by reduction leaving MG(KJ)
d_{tg}	Sensible heat loss by top gas (KJ)
$d_{cooling}$	Sensible heat loss during cooling of reduction gas (KJ)
d_{out}	Sensible heat loss due to reduction gas taken out of the process (KJ)
S_{PC}	Heat supplied by post combustion (KJ)
S_{coal}	Heat supplied by coal combustion (KJ)
S_{total}	Total heat supplied (KJ)
D_{total}	Total heat demand (KJ)
n_C^A	kg moles of C reacting with oxygen
n_C^r	kg moles of C leaving MG in the reduction gas
n_C^{rg}	kg moles of C leaving in the reduction gas taken out of the process
n_H^{rg}	kg moles of H leaving in the reduction gas taken out of the process
n_N^{rg}	kg moles of N leaving in the reduction gas taken out of the process
$(O/C)^{rg}$	kg moles of O per kg mole of C leaving in the reduction gas taken out of the process
$(O/C)^{tg}$	kg moles of O per kg mole of C in the top gas
$(O/H_2)^{rg}$	kg moles of O per kg mole of H_2 in the reduction gas taken out of the process
$(O/H_2)^{tg}$	kg moles of O per kg mole of H_2 in the top gas
(O/Fe)	kg moles of O per kg mole of iron in the iron oxide.
n_O^B	kg moles of O injected for coal combustion
n_O^{add}	kg moles of secondary O injected for post-combustion
n_{Si}^a	kg moles of SiO_2 from ore joining hot metal as Si
$n_{SiO_2}^b$	kg moles of SiO_2 in slag from ore

n_{Si}^c	kg moles of SiO_2 from coal ash joining hot metal as Si
$n_{SiO_2}^d$	kg moles of SiO_2 from coal ash joining slag
n_{Si}^a	kg moles of S in HM from ore
n_{CaS}^b	kg moles of S from coal joining slag as CaS
n_S^c	kg moles of S in HM from coal
n_{CaS}^d	kg moles of S in coal joining slag as CaS
$n_{CO}^r, n_{CO_2}^r, n_{H_2O}^r, n_{H_2}^r, n_{N_2}^r$	kg moles of respective component of reduction gas leaving the MG
$n_{CO}^{ro}, n_{H_2}^{ro}, n_{H_2O}^{ro}, n_{CO_2}^{ro}, n_{N_2}^{ro}$	kg moles of respective component of reduction gas taken out of the process
$n_{CO}^{tg}, n_{CO_2}^{tg}, n_{H_2O}^{tg}, n_{H_2}^{tg}, n_{N_2}^{tg}$	kg moles of respective component of top gas

ppc	percentage post-combustion
T_M	temperature of hot metal (K)
T_R	temperature of reduction gas leaving MG (K)
T_C	temperature of reduction gas after cooling (K)
T_g	temperature of top gas (K)
X	degree of metallization
MG	Melter - gasifier
RSF	Reduction shaft furnace

CHAPTER - 1

INTRODUCTION

In the past few decades, the blast furnace has attained a level of perfection which led to an essential increase in production, improvement in quality and reduction in consumption of coke. However, for the blast furnace, the price that is paid for perfection is the preparation of input materials as coal and ore fines cannot be charged there. Coal requires to be converted into hard coke and ore fines need to be converted into sinter or pellets before they can be charged into the furnace.

In the production of sinter and coke it is very difficult to take care of the environmental problems. Scarcity of coking coal reserves is another problem. So, any effort to reduce the coking coal consumption is welcome in the steel industry. Many advances have been made in the area of reducing coke consumption in the blast furnace : they are oxygen enrichment, fuel injection, blast humidification, use of self and superfluxed sinter/pellets, high top pressure, coal injection in the blast furnace etc. Amongst them coal injection through blast furnace tuyeres is the recent one which resulted in the significant reduction in coke rate. Though reduction in coke rate is achieved, but the blast furnace cannot work without coke because it needs a coke grid in hearth and bosh to support burden and "coke - windows" in the cohesive zone in order to maintain satisfactory gas permeability in this area [14].

The emphasis on the use of coal as received from mines and

iron ore fines and to restrict the installation of new coke ovens led to the development of direct reduction and smelting reduction. Direct reduction processes employ gas or coal for the reduction of iron ore to sponge iron in the solid state. Sponge iron is smelted in electric arc furnace to get hot metal. The process has some disadvantages which still stop its breakthrough :

After reduction, sponge iron has to be protected against reoxidation and for smelting of sponge iron to hot metal very expensive and short supply of electric power is required, so that the process remains uneconomical.

The smelting reduction processes are paid much attention as a possible alternative to overcome the limitations of the blast furnace and direct reduction processes. The smelting reduction processes aim at using the fine ore and wide range of coal without much preparation. The direct use of coal in smelting reduction produces large amount of reducing gases. It requires a combination of final reduction and melting in or directly above the iron both, with the use of produced gases for pre-reduction. The advantages of smelting reduction process over the other ironmaking process can be defined as follows [4,7,15] :

- The process is coal-based with no restriction to its grade.
- The process does not require the preparation of input materials as ore fines and coal can be charged here. In this way, the emission of air pollutants during sintering and coking can be avoided. So, the process is environment friendly also.
- The economy of the process does not depend on the surplus gas

production i.e. if demand for surplus gas is not there, the gas is utilized in the process itself.

- Investment cost is lower because making coking oven and agglomeration plants is unnecessary here. Space requirement is also reduced due to this.
- Many smelting reduction processes employ a fluidized bed [16] for pre-reduction of iron ore because fluidized bed is ideal for the reduction of iron ore. Large surface area ensures good conditions for reduction.

Due to high thermal efficiency obtained in the blast furnace smelting reduction processes cannot pose a challenge to the blast furnace, but non-availability of coking coal and environment problems are the factors which cannot be dispensed with. So, there is a lot of scope for development in smelting-reduction processes.

Two-stage smelting reduction process is the most efficient one among the smelting reduction processes for ironmaking because off-gas can be used for pre-reduction within the process itself. The seven COREX plants (a two-stage smelting reduction process), under operation or construction will upon completion in the year 1998, feature a total production capacity of nearly 5 million tonnes of hot metal per year.

India has also progressed in this area by setting up two COREX plants at Jindal Toranagallu Works which are scheduled to start production in October 1997 and March 1998 respectively.

Since in the current ironmaking scenario the two-stage smelting reduction process has gained a lot of importance, the

objective of the present work is to model such a process thermo-chemically so as to get information about it. Main smelting reduction processes are discussed in chapter two. The chapter emphasizes the emerging need for the two-stage smelting reduction process which is modelled in chapter three. Chapter four discusses the results obtained from the model. Here the model for the two stage smelting reduction process has also been extended to blast furnace process. Finally, chapter five outlines the conclusions and chapter six scope for the further work in this area.

CHAPTER - 2

LITERATURE SURVEY

The smelting reduction processes are paid much attention as a possible alternative to overcome the limitations of the blast furnace and direct reduction processes [19]. Blast furnace requires coke and sintered/pelletized iron ore for smooth and successful operation. The coking coal reserves are scarce and the processes for sinter and pellet making are not very much environmental friendly. Direct reduction process produce sponge iron which needs proper handling. Moreover, these processes do not produce liquid iron as that of blast furnace.

In last seventies and early eighties, concerted efforts were made in many parts of the world to develop a process of making liquid iron similar to blast furnace hot metal (and not sponge iron) using non-coking coal. These new processes are termed as smelting reduction processes. They aim at using fine ore and wide range of coal grades directly. Here a substantial part of the reduction takes place in the liquid oxide phase [19]. The direct use of coal in smelting reduction produces large amount of reducing gases. Many smelting reduction processes employ a fluidized bed for pre-reduction of iron ore because fluidized bed is ideal for the reduction of iron ore [16]. So, agglomeration of burden is no more required.

2.1 THERMOCHEMICAL CONFIGURATIONS FOR SMELTING REDUCTION [7,18]

Based on the flow of material and heat, the following thermochemical configurations can be conceptually realized for smelting reduction processes:

(a) Single stage process

- (b) Two stage process
- (c) Three stage process

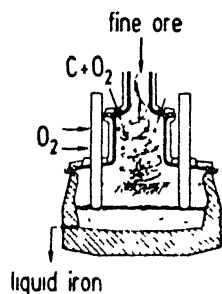
2.1.1 Single Stage Process

The simplest reactor configuration is a single well stirred vessel in which cold ore, fuel and oxygen are reacted (see Fig. 2.1). The metal and off gases are produced at about 1650°C and the off gas contains high calorific value reducing gas ($\text{CO} + \text{H}_2$).

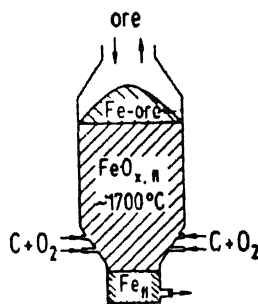
A single stage smelting - reduction process is extremely inefficient and is not technically or economically high temperature. So, large amount of sensible heat is also carried away with it. This is shown in Table 2.1 for various coals.

Table 2.1: Top gas sensible heat and calorific value for various coals [18]

Fuel (Dry ash free)	Top gas	
	Sensible Heat (GJ)	Calorific Value (GJ)
C	8.4	43.9
Bituminous coal	12.4	63.6
Sub-bituminous coal	16.4	84.0



with electrical energy



with coal

Fig. 2.1 : Principles of single-stage smelting reduction process

Unless adequate demand for large amount of high calorific value top gas is not there, this process will not remain economically viable.

2.1.2 TWO-STAGE PROCESS

The obvious improvement to the single-stage process is to utilize the melter off gases for pre-reduction, thereby reducing the energy requirement in the melter to that for melting and final reduction and usefully employing part of the chemical energy in the off - gases within the process. This concept has been shown in Fig. 2.2.

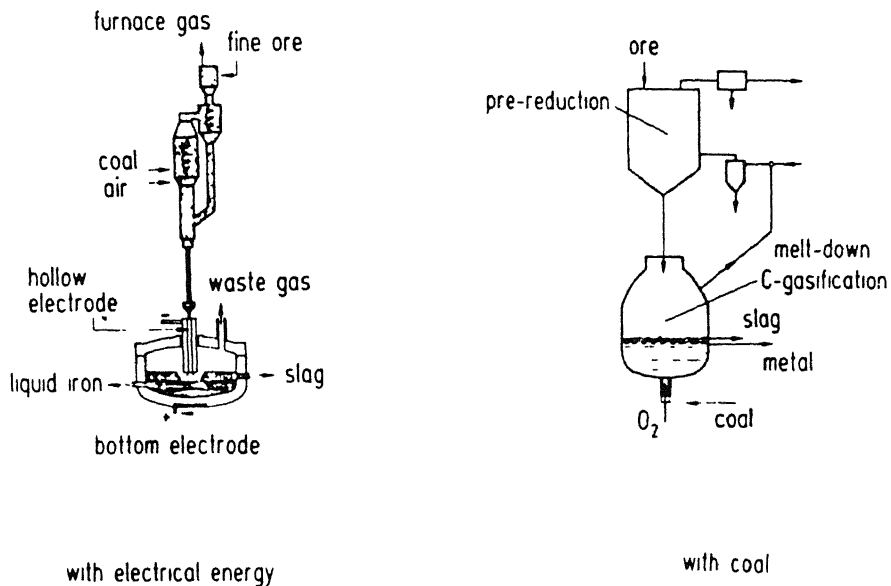


Fig. 2.2 : Principles of two-stage smelting reduction process

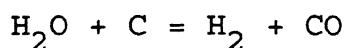
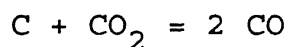
In an integrated process of this nature, it is fundamental to match the performance of the two operations. One possible way of operating the process is to ensure by control of the melting process that off-gas make matches the requirement to produce highly metallized ore [8].

For reduction to a higher degree of metallization using reduction gas, its calorific value should be high in order to meet thermodynamic and process constraints which apply during the reduction of iron ore. Since the utilization of CO and H₂ for wustite - iron equilibrium at 1200 K is 30% and 37% respectively. The top gas will still have very high calorific value. Since pure O₂ is used for coal combustion here, very less amount of N₂ (coming from coal) will be available in the top gas. The rejection of energy in the top gas can be avoided by the removal of CO₂ and H₂O from it and recycling the gas through the pre-reduction unit. By this means it is possible to conserve chemical energy value of the reducing species in the spent reducing gas, but energy is required to remove CO₂ and H₂O and to compress and reheat the recycled gas. But it is worth noting that the energy consumption for recycle operation is significantly greater than the once through process under conditions where the top gas energy is used effectively [18]. So, it is always advantageous to produce DRI in a separate facility by utilizing the top gas for the reduction work [7]. It is obvious that the energy consumption for the two - stage smelting reduction process is significantly superior to the single stage process. However, the contains two inherent sources of heat rejection. The first one is the cooling of reduction gas and the second is that from top gas leaving the reduction shaft. The three stage smelting reduction process aim to utilize these sources of heat.

2.1.3 Three - Stage Process

The interposition of a reaction zone containing free carbon between the melting and reduction zones provides a means of

reducing the temperature of the melter off gas, without rejection of energy, through the reactions:



These reactions are both highly endothermic and effectively provide a mechanism whereby excess sensible heat in the gas can be converted to chemical energy available for reduction. The thermodynamics of the carbon-oxygen system impose a lower limit of temperature which can be reached by gasification reaction. The various types of three-stage processes are shown in Fig. 2.3. The third stage typically consists of a bed on carbon access material

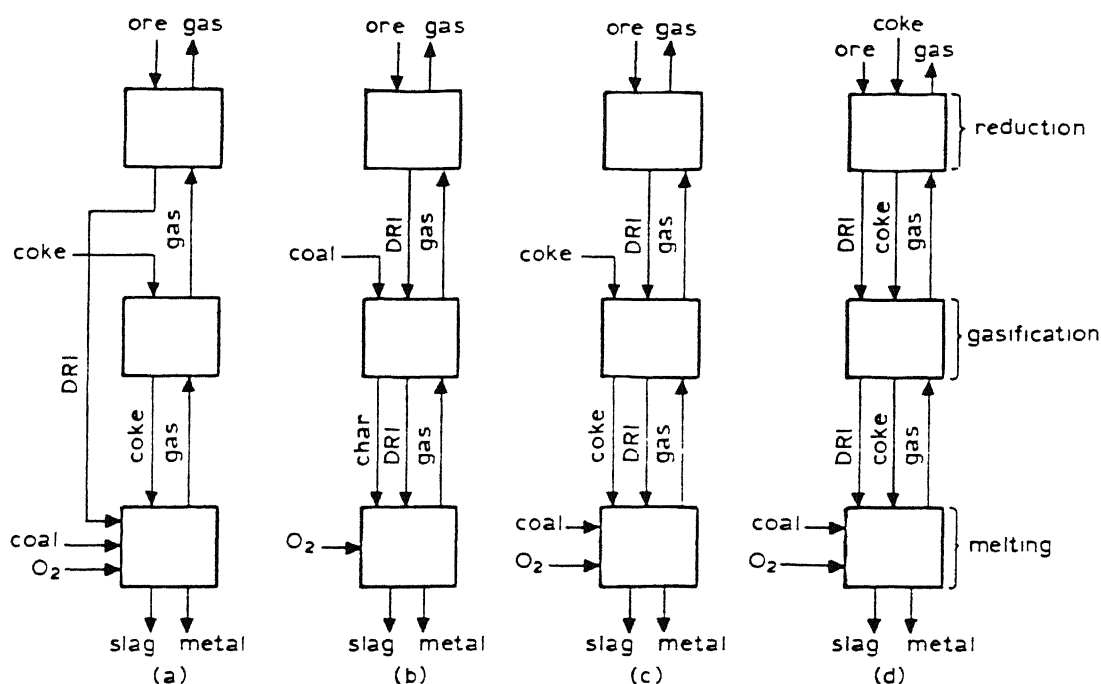


Fig. 2.3 : Principles of three-stage smelting reduction process

and in practice it is not necessarily separated from the melting reactor and in melters based on a coke bed the gasification reactions will take part in the upper portion of the melting reactor.

The incorporation of the third stage results in a process with lower energy consumption. Since in the category coke is used in the production of hot metal, the limitations of the blast furnace to use scarce coking coal is valid here also. Energy associated with coking of coal makes the overall energy consumption higher.

2.2 TECHNO-ECONOMIC VIABILITY [16,18]

The energy consumption in iron production for all three configurations has been given in Table 2.2. Single - stage process is significantly worse than the other processes and this process is of interest where there is a local customer with a large requirement for high calorific value gas.

A dramatic improvement is achieved by the two stage process by utilizing the reduction gas within the process itself. For three-stage smelting reduction process, the energy consumption is still lower. But the biggest disadvantage of this process is that it uses coke. In view of scarcity of coking coal, making coke-ovens and environmental problems, three-stage smelting reduction process cannot be taken as techno-economically viable in the current ironmaking scenario.

The energy costs for three - stage processes utilizing coke are somewhat higher than the two stage process because of the cost differential between coal and coke [18]. So the only process which sounds to be techno-economic viable is the two-stage

**Table 2.2 : ENERGY CONSUMPTION FOR THE THREE CONFIGURATIONS AND
THE BLAST FURNACE FOR IRON PRODUCTION (GJ/thm) [18]**

Process Type	Net Energy Consumption
Single Stage	26.5 - 29.9
Two Stage	15.5 - 16.5
Three Stage a & c	13.9 - 14.5
b	13.5 - 13.9
d	13.3 - 13.6
Blast furnace	14.7

smelting reduction process.

Various smelting reduction processes can be categorised into the three stages described above. This categorization has been shown in Table 2.3.

Table 2.3 : Smelting reduction processes [18]

SINGLE STAGE	TWO STAGE	THREE STAGE
COIN PROCESS	COREX PROCESS	KAWASAKI PROCESS
BSC PROCESS	XR PROCESS	PLASMA SMELT PROCESS
HOOGOSENS PROCESS	INRED PROCESS	KORF-KR PROCESS
HISMELT PROCESS	ELRED PROCESS	SUMITOMO-SC PROCESS
CIG PROCESS	COMBISMELT PROCESS	
KOBE PROCESS		
BSC-ICI PROCESS		
NIPPON-STEEL PROCESS		

Until now, there is only one operational realization of the two stage smelting reduction process which is the COREX process developed by Voest Alpine of Austria.

Other smelting reduction technologies will not become commercially viable with in this decade.

2.3 COREX PROCESS DESCRIPTION [7,10,15,19]

Fine ore is first charged into a reduction shaft via a lock hopper system where they are reduced to approximately 90% metallized directly reduced iron by a reduction gas moving in counter flow (see Fig. 2.4). Discharge screw conveys the directly reduced iron from the reduction shaft into the so called melter gasifier where final reduction of directly reduced iron takes place. Hot metal and slag are tapped at around 1500-1600°C as in conventional blast furnace. Viewing the process from the coal route, non-metallurgical coal is directly charged into the melter-gasifier via a lock hopper system. Combustion with pure O_2 in melter-gasifier results in generation of highly efficient reduction gas. Due to high temperature pre-dominating in the dome of MG (in excess of 1000°C), the higher hydrocarbons released from coal during devolatilisation are immediately dissociated to CO and H_2 . Undesirable products such as tars, phenols etc are destroyed and cannot be released to atmosphere.

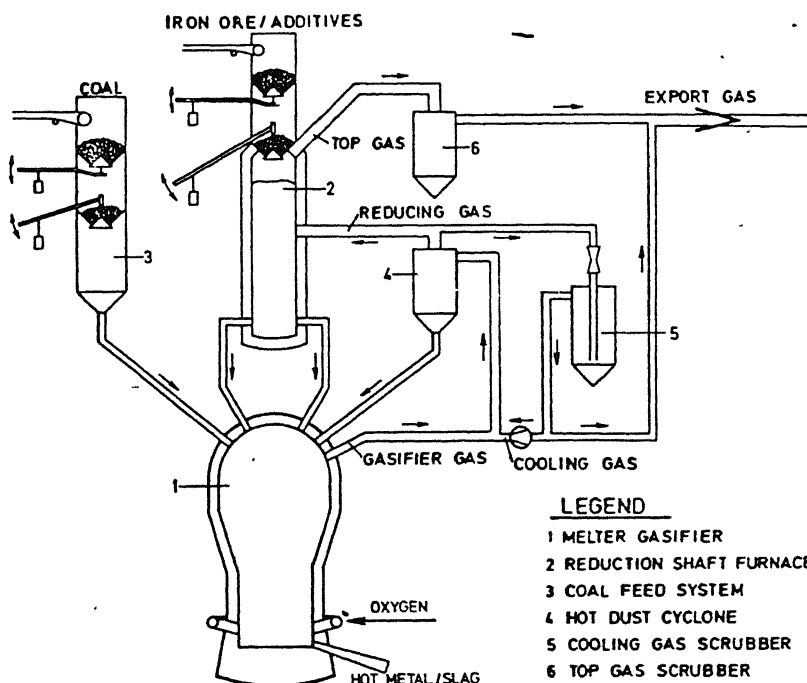


Fig. 2.4 COREX process flow sheet

The reduction gas leaving MG consists of CO and H₂ laden with fine coal, ash and iron dust. This dust is removed in a hot gas cyclone. Through the addition of cooling gas, the reduction gas temperature is adjusted to about 800-850°C. After leaving the hot gas cyclone the reduction gas is then blown into the reduction shaft via a bustle, reducing the iron ores in counter flow.

The top gas is subsequently cooled and cleaned in a scrubber, after which it is available as a highly calorific value export gas suitable for wide range of applications:

- power generation
- production of DRI
- saleable high CV gas
- heating purpose in an iron and steel complex.

2.4 COREX PLANTS [7,19]

There are seven COREX plants in operation or under construction which upon completion in the year 1998 will have a production capacity of about 5 million tonnes.

2.4.1 In Operation

- (a) ISCOR Pretoria Works (South Africa)

Operating since 1989

Capacity = 1000 thm/day

- (b) POSCO Pohang Works (South Korea)

Operating since November 1995

Capacity = 2000 thm/day

2.4.2 Under Construction

- (a) HANBO Dangjin Works (Asan Bay, Korea)

Two plants will become operational in 1998.

Total Capacity = 2 million thm/annum

The export gas produced will be used for the production of DRI in a separated MIDREX facility.

(b) JINDAL Toranagallu Works, India

Two plants will become operational in October, 1997 and March, 1998 respectively.

Total Capacity = 1,530,000 thm/annum

Export gas generated will be used to run two power plants and a pelletizing plant.

(c) Suldanha Steel Works (South Africa)

It will become operational in 1998.

Capacity = 650,000 thm/annum

Export gas will be used to for the production of DRI in a separate facility.

2.5 COREX vs. BLAST FURNACE [7,16]

COREX	Bf/C
Export gas (high CV)	Top gas (low CV)
Less energy consumption <ul style="list-style-type: none"> ■ No burden preparation ■ Post-combustion ■ Post-combustion 	High energy consumption <ul style="list-style-type: none"> ■ Coke ovens ■ Sintering ■ Nopost combustion
No Blast temperature (Pure O ₂ used)	Blast Temperature (Air is used)
No injectants through injected O ₂	Injectants (Like H ₂ O, O ₂ , HC) through air blast
Less Polluting	More polluting
Low capital cost	High capital cost
Less space requirement	More space requirement
More flexible	Less flexible

2.6 OBJECTIVES OF THE PRESENT STUDY

In the present study a thermochemical model of the two stage

of smelting - reduction has been prepared to investigate the process - technological parameters influencing the corex process for ironmaking. Separate materials and heat balance are made for reduction shaft and melter - gasifier. Two cases are considered; in one, thermal and chemical demand for reduction shaft and melter-gasifier is met by coal combustion and in the other thermal and chemical demand for melter-gasifier is met by coal combustion and that of reduction shaft from other source of energy. For both the cases, a computer programme is developed to investigate the influence of degree of metallisation, post combustion ratio, amount of slag and coal grade on the following (all per ton of hot metal).

- i. Coal consumption
- ii. Oxygen requirements for combustion of coal and post combustion
- iii. Reduction gas amount and its composition
- iv. Surplus energy
- v. Top gas amount and its composition.

For the above calculations, the following input variables are fixed.

- i. composition of hot metal, slag and ash
- ii. tapping temperature of hot metal and slag
- iii. reduction shaft and top gas temperature
- iv. temperature of reduction gas existing melter gasifier
- v. limestone contains only CaCO_3
- vi. heat losses due to radiation and convection

The model is extended to blast furnace ironmaking and some results are also presented.

CHAPTER - 3

THERMO-CHEMICAL MODEL

A thermo-chemical model needs complete heat and materials balance of the process. The model is developed by first preparing the materials - balance equations for the process. Then heat demand and supply terms are formulated mathematically and are equated to give heat balance equation. Finally heat and materials balance equations are coupled to form the model.

Ultimate objective of the model development for two stage smelting reduction process is to provide following information:

1. Coal consumption
2. Oxygen requirement for coal combustion and post combustion
3. Reduction gas amount and composition
4. Surplus gas calorific value
5. Top gas amount and composition

3.1 PROCESS DESCRIPTION [7,20]

Two stage smelting reduction process consists of two reactors. The first reactor, where iron ore pre-reduction is done, is called the 'reduction shaft furnace' whereas the second one, in which smelting - reduction of pre-reduced iron ore to hot metal, production of reduction gas and slag are carried out, is known as the 'melting-gasifier'.

Iron ore fines and limestone are charged into the reduction shaft furnace where iron ore is pre-reduced by a highly efficient reducing gas (known as the 'reduction gas') coming at around 1300 K from the melting-gasifier [7].

Pre-reduced ore and limestone from the reduction shaft

furnace at around 1200 K are conveyed into the melter-gasifier whereas coal is directly charged into it. Here, final reduction of pre-reduced ore takes place in addition to decomposition of CaCO_3 , reduction of oxides, drying and devolatilization of coal and slag reactions. Combustion of coal with pure oxygen injected into the melter-gasifier results in the generation of a highly efficient reduction gas. Hot metal and slag are tapped at around (1700 - 1850 K).

The reduction gas leaves the melter gasifier laden with dust fines. This dust is largely removed from the gas stream in a hot gas cyclone and after adjusting the temperature to around 1250 K [7], the reduction gas is then blown into the reduction shaft via a bustle pipe for reducing iron ore in counter flow. The reduction gas may be post combusted [1] in the melter-gasifier by supplying extra oxygen from top of the melter-gasifier. The combustion of reduction gas will lead to generation of heat which in turn would help in saving of coal. The concept of post combustion is not yet applied in the COREX process but has significant potential in the COREX process technology.

The top gas, which consists of CO , CO_2 , H_2 , H_2O and N_2 , leaves the reduction shaft furnace at around 500 - 800 K [18]. The top gas and the surplus reduction gas are subsequently cooled and cleaned in a scrubber after which it is available for wide range of applications such as power generation, sponge iron production etc. The cooled and cleaned gas is called the 'export-gas'.

For the minimum consumption of coal, there should not be an excess production of reduction gas i.e. production of reduction

gas in melter-gasifier should be sufficient to meet the requirement of pre-reduction in the reduction shaft furnace. This requirement will lead to certain fixed degree of pre-reduction of iron ore which is known as 'optimum pre-reduction (or optimum metallization) [8].

3.2 MODEL FORMULATION

Model to be developed for two stage smelting reduction process has been formulated by incorporating assumptions into the actual process.

3.2.1 Assumptions

Following assumptions are made:

- (1) Process is operating at steady state
- (2) Metallized ore and CaCO_3 leave the reduction shaft furnace at 1200 K and there occurs no decomposition of CaCO_3 in the reduction shaft furnace (i.e. below 1200 K) [14].
- (3) The combustion efficiency of coal is 100% and no loss of coal particles occur. In the melter-gasifier, the fluidized bed process for combustion of coal is employed. The efficiency of such a process of combustion is normally very high [16]. Loss of fines also occurs during fluidized bed combustion. Most of these fines are circulated back into the melter-gasifier through the use of hot dust cyclone.
- (4) Iron entering the process from sources other than ore is too small to be neglected. No FeO in slag is considered.
- (5) Pure CaCO_3 is considered for calculations.

3.2.2 Flow of the Materials

The flow of materials is shown in Fig. 3.1.

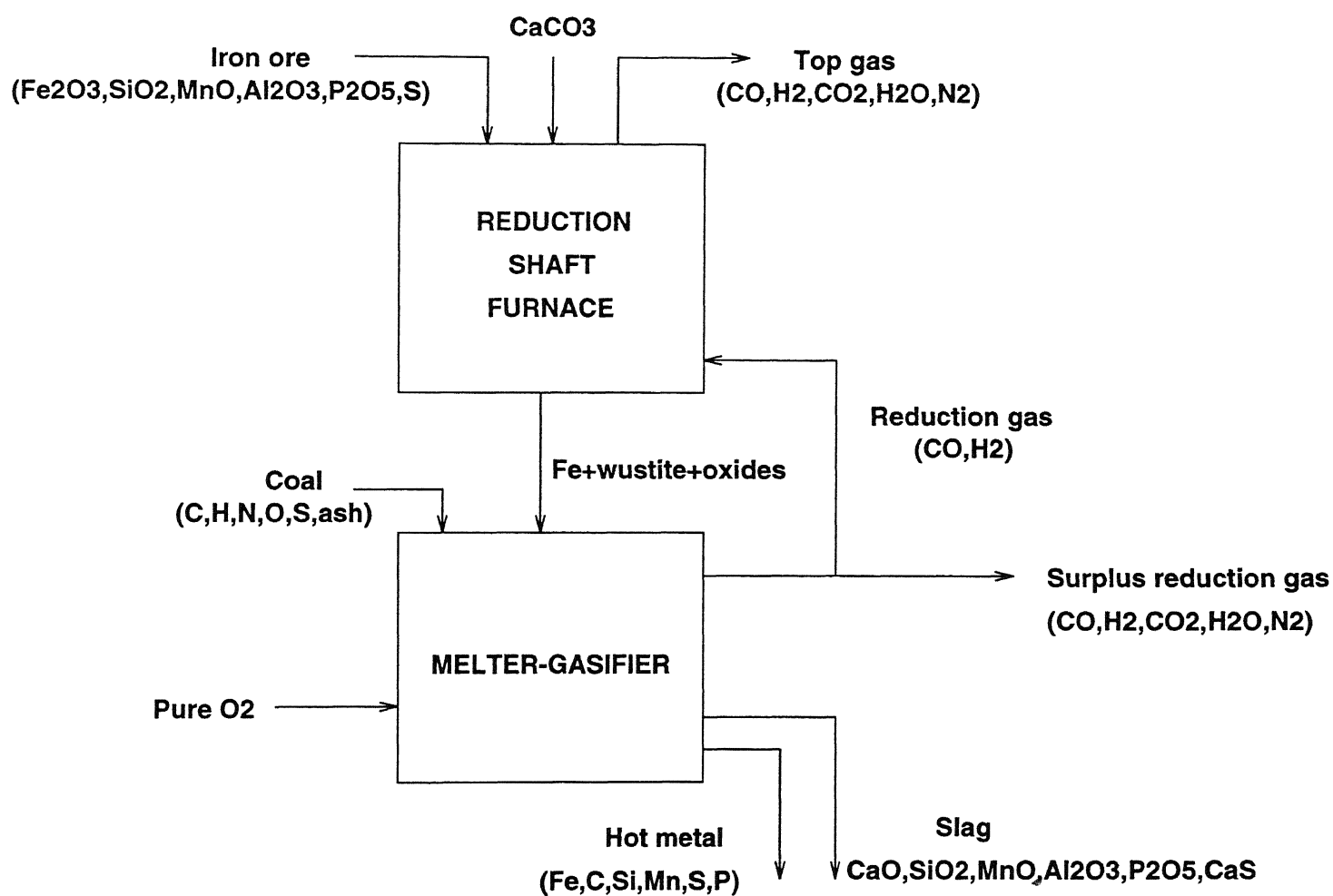


FIG.3.1 : THE FLOW OF MATERIALS IN THE THE TWO-STAGE SMELTING REDUCTION PROCESS

3.3 Materials Balance

Since hot metal and slag consist of elements and oxides respectively, elemental balances for C, Fe, Si, Mn, S, P, H, N, O and Ca and oxide balance for Al_2O_3 have been carried out separately. Calculations for C/Fe, Si/Fe, Mn/Fe, S/Fe, P/Fe, n_{CaO} , n_{SiO_2} , $n_{\text{Al}_2\text{O}_3}$ and n_{CaS} are given in appendix III.

3.3.1 C-Balance

Carbon comes into the process from coal and CaCO_3 (1 kg mole of CaCO_3 on decomposition gives 1 kg mole of CO_2 , so in carbon balance it will account for 1 kg mole of carbon in).

So,

$$n_C^i = n_C^{\text{coal}} + n_{\text{CaCO}_3} \quad (3.3)$$

$$\text{where } n_C^{\text{coal}} = \frac{C_x (\% \text{C in Coal})}{12 \times 100} \quad (3.4)$$

Carbon leaves the process in the hot metal as C, in reduction gas taken out of the process and top gas as CO and CO_2 which means,

$$n_C^o = n_C^{\text{tg}} + n_C^{\text{rg}} + (\text{C/Fe}) \quad (3.5)$$

$$\text{Now } n_C^{\text{tg}} = C_{\text{reduction gas with PC}} + C_{\text{reduction gas without PC}} - n_C^{\text{rg}} \quad (3.6)$$

(Dust losses and carbon deposition in reduction shaft are assumed to be negligible).

$$\text{Then } n_C^A = n_C^{\text{tg}} + n_C^{\text{rg}} \quad (3.7)$$

$$\text{At steady state, } n_C^i = n_C^o \quad (3.8)$$

Combining equations (3.3) - (3.8), we get

$$n_C^A = \frac{C_x (\% \text{C in coal})}{1200} + n_{\text{CaCO}_3} - (\text{C/Fe}) \quad (3.9)$$

3.3.2 Fe-Balance

Fe enters the reactor as Fe_2O_3 in the iron ore and it leaves as Fe in the hot metal. Fe entering from other sources and leaving as FeO in slag is too small to be neglected. Since our basis of calculations is 1 kg mole of product Fe, we have

$$n_{\text{Fe}}^i = n_{\text{Fe}}^o = 1 \quad (3.10)$$

Iron ore undergoes metallization in the reduction shaft furnace (= X%, say) by reduction gas coming from melter-gasifier. Iron will come out of the reduction-shaft as $\text{Fe}_{0.95}\text{O}$ and Fe (if amount and composition are maintained in the reduction shaft corresponding to wustite - Fe equilibrium). The mixture of $\text{Fe}_{0.95}\text{O}$ and Fe further changes to liquid iron in the melter-gasifier.

$$\text{This means, } n_{\text{Fe}} + 0.95 n_{\text{Fe}_{0.95}\text{O}} = 1 \quad (3.11)$$

$$\% \text{ Metallization (X)} = \frac{n_{\text{Fe}} \times 100}{n_{\text{Fe}} + 0.95 n_{\text{Fe}_{0.95}\text{O}}} \quad (3.12)$$

Substituting (3.11) in (3.12), we get

$$n_{\text{Fe}} = \frac{X}{100} \quad (3.13)$$

and substituting (3.13) in (3.11), we get

$$n_{\text{Fe}_{0.95}\text{O}} = \left(\frac{100 - X}{95} \right) \quad (3.14)$$

3.3.3 Si - Balance

Si enters the process as SiO_2 from iron ore and coal ash whereas it leaves as Si in the hot metal and as SiO_2 in the slag.

$$\text{So, } n_{\text{Si}}^i = n_{\text{SiO}_2}^{\text{coal}} + n_{\text{SiO}_2}^{\text{ore}} \left(\text{One kg mole of SiO}_2 \text{ corresponds to one kg mole of Si} \right) \quad (3.15)$$

$$\text{where } n_{\text{SiO}_2}^{\text{coal}} = \frac{C_x \left(\frac{\% \text{ ash in}}{\text{coal}} \right) \left(\frac{\% \text{ SiO}_2 \text{ in}}{\text{ash}} \right)}{100 \times 100 \times 60} \quad (3.16)$$

$$\text{Also, } n_{\text{Si}}^{\text{O}} = \left(\text{Si/Fe} \right) + n_{\text{SiO}_2} \quad (3.17)$$

$$\text{at steady state, } n_{\text{Si}}^{\text{i}} = n_{\text{Si}}^{\text{O}} \quad (3.18)$$

using equations (3.15) - (3.18), we get

$$n_{\text{SiO}_2}^{\text{ore}} = \left(\text{Si/Fe} \right) + \left(n_{\text{SiO}_2} \right) - \frac{C_x \left(\frac{\% \text{ ash in}}{\text{coal}} \right) \left(\frac{\% \text{ SiO}_2 \text{ in}}{\text{ash}} \right)}{100 \times 100 \times 60} \quad (3.19)$$

3.3.4 Mn - Balance

Mn enters the process as MnO in iron ore and leaves as Mn in the hot metal and as MnO in the slag. At steady state,

$$n_{\text{Mn}}^{\text{i}} = n_{\text{Mn}}^{\text{O}} \quad (3.20)$$

$$n_{\text{Mn}}^{\text{O}} = (\text{Mn/Fe}) + n_{\text{MnO}} \quad (3.21)$$

1 kg mole of MnO corresponds to one kg mole of Mn.

$$n_{\text{Mn}}^{\text{i}} = n_{\text{MnO}}^{\text{ore}} \quad (3.22)$$

3.3.5 S - Balance

Sulphur enters the process from iron ore and coal. It leaves as S in the hot metal and as CaS in the slag. In the iron ore S is considered to be present as FeS. The mass balance of S is

$$n_{\text{S}}^{\text{i}} = n_{\text{FeS}}^{\text{ore}} + n_{\text{S}}^{\text{coal}} \quad (3.23)$$

(1 kg mole of FeS corresponds to 1 kg mole of sulphur)

$$\text{where } n_{\text{S}}^{\text{coal}} = \frac{C_x \left(\frac{\% \text{ S in}}{\text{coal}} \right)}{32 \times 100} \quad (3.24)$$

$$\text{Also, } n_{\text{S}}^{\text{O}} = (\text{S/Fe}) + n_{\text{CaS}} \quad (3.25)$$

(1 kg mole of CaS corresponds to 1 kg mole of S)

$$\text{At steady state, } n_S^i = n_S^o \quad (3.26)$$

Combining (3.23) - (3.26), we get,

$$n_{\text{FeS}}^{\text{ore}} = \left(\text{S/Fe} \right) + n_{\text{CaS}} - \frac{C_x \left(\frac{\% \text{ S in}}{\text{coal}} \right)}{32 \times 100} \quad (3.27)$$

3.3.6 P - Balance

Phosphorus enters the process as P_2O_5 in iron ore and leaves as P in the hot metal.

At steady state, we have

$$n_P^i = n_P^o \quad (3.28)$$

$$\Rightarrow n_P^o = \left(\text{P/Fe} \right) \quad (3.29)$$

$$n_P^i = 2 n_{\text{P}_2\text{O}_5}^{\text{ore}} \quad (3.30)$$

(1 kg mole of P_2O_5 corresponds to 2 kg moles of phosphorus)

3.3.7 Hydrogen Balance

Hydrogen comes into the process from volatile matter and moisture in coal. Hydrogen leaves the process as H_2 and H_2O in the top gas and reduction gas out of the process before it enters the reduction shaft furnace.

$$\text{At steady state, } n_H^i = n_H^o \quad (3.31)$$

$$n_H^i = n_H^o = \left[\frac{C_x \left(\frac{\% \text{ H in}}{\text{coal}} \right)}{100} + 2 \left(\frac{C_x \left(\frac{\% \text{ moisture in}}{\text{coal}} \right)}{18 \times 100} \right) \right] \quad (3.32)$$

(1 kg mole of H_2O corresponds to 2 kg moles of H)

$$\text{Also, } n_H^o = n_H^{\text{rg}} + n_H^{\text{tg}} \quad (3.33)$$

3.3.8 Nitrogen Balance

Since pure oxygen has been supplied for combustion of coal and post-combustion of reducing gases, nitrogen enters the process as N in coal only whereas it leaves the process as N_2 in the

reduction gas taken out of the process and top gas. N_2 , because of its inert nature, does not participate in any reaction of the process. It merely acts as heat carrier gas.

$$n_N^i = \frac{C_x \left(\frac{\% N \text{ in coal}}{14 \times 100} \right)}{14 \times 100} \quad (3.34)$$

$$\text{And } n_N^o = n_N^{rg} + n_N^{tg} \quad (3.35)$$

$$\text{At steady state, } n_N^i = n_N^o \quad (3.36)$$

3.3.9 Oxygen Balance

Oxygen enters the process as the oxygen injected for coal combustion, as oxygen injected for post-combustion of reducing gases, iron oxide, other oxides (on reduction 1 kg mole of SiO_2 gives 2 kg moles of O, 1 kg mole of MnO on reduction gives 1 kg mole of O, one kg mole of P_2O_5 gives 5 kg moles of O and two kg moles of P (i.e. 2.5 kg moles of O per kg mole of P), $CaCO_3$ (one kg mole of $CaCO_3$ on decomposition gives two kg moles of O), coal moisture (1 kg mole of H_2O gives one kg mole of O) and coal oxygen.

$$\begin{aligned} \text{So, } n_O^i &= n_O^B + n_O^{add} + \left(O/Fe \right) + 2 \left(Si/Fe \right) \\ &+ \left(Mn/Fe \right) + 2.5 \left(P/Fe \right) + 2 n_{CaCO_3} \\ &+ \frac{C_x \left(\frac{\% \text{ moisture in coal}}{18 \times 100} \right)}{18 \times 100} + \frac{C_x \left(\frac{\% O \text{ in coal}}{16 \times 100} \right)}{16 \times 100} \end{aligned} \quad (3.37)$$

Since iron oxide enters the process as Fe_2O_3 , so $O/Fe = 1.5$ in equation (3.37).

$$\begin{aligned}
 \text{i.e } n_O^i &= n_O^B + n_O^{\text{add}} + 1.5 + 2 \left(\text{Si/Fe} \right) + \left(\text{Mn/Fe} \right) \\
 &+ 2.5 \left(\text{P/Fe} \right) + 2n_{\text{CaCO}_3} \\
 &+ \frac{C_x \left(\begin{array}{c} \% \text{ moisture} \\ \text{in coal} \end{array} \right)}{1800} + \frac{C_x \left(\begin{array}{c} \% \text{ O in} \\ \text{coal} \end{array} \right)}{1600}
 \end{aligned} \tag{3.38}$$

Oxygen leaves the process in the reduction gas taken out of the process before it enters the reduction shaft furnace and in the top gas as CO , CO_2 and H_2O .

So,

$$\begin{aligned}
 n_O^O &= \left(\text{O/C} \right)^{\text{rg}} \cdot n_C^A + \left(\text{O/H}_2 \right)^{\text{rg}} \cdot n_{\text{H}_2}^O \\
 &+ \left(\text{O/C} \right)^{\text{tg}} \cdot n_C^A + \left(\text{O/H}_2 \right)^{\text{tg}} \cdot n_{\text{H}_2}^O
 \end{aligned} \tag{3.39}$$

$$\text{where } n_H^O = 2 n_{\text{H}_2}^O \tag{3.40}$$

Determination of $\left(\text{O/C} \right)^{\text{rg}}$, $\left(\text{O/C} \right)^{\text{tg}}$, $\left(\text{O/H}_2 \right)^{\text{tg}}$ and $\left(\text{O/H}_2 \right)^{\text{rg}}$ is given in the appendix IV.

Now at steady state,

$$n_O^i = n_O^O \tag{3.41}$$

Combining (3.38), (3.39) and (3.41), we get

$$\begin{aligned}
 n_O^B &= \left(\text{O/C} \right)^{\text{rg}} \cdot n_C^A + \left(\text{O/C} \right)^{\text{tg}} \cdot n_C^A + \left(\text{O/H}_2 \right)^{\text{tg}} \cdot n_{\text{H}_2}^O \\
 &+ \left(\text{O/H}_2 \right)^{\text{rg}} \cdot n_{\text{H}_2}^O - n_O^{\text{add}} - 1.5 - 2 \left(\text{Si/Fe} \right) - \left(\text{Mn/Fe} \right) \\
 &- 2.5 \left(\text{P/Fe} \right) - 2n_{\text{CaCO}_3} \\
 &- \frac{C_x \left(\begin{array}{c} \% \text{ moisture} \\ \text{in coal} \end{array} \right)}{1800} - \frac{C_x \left(\begin{array}{c} \% \text{ O in} \\ \text{coal} \end{array} \right)}{1600}
 \end{aligned} \tag{3.42}$$

Since post-combustion of 1 kg mole of CO to CO_2 and 1 kg mole of H_2 to H_2O both require one kg mole of O each.

$$\text{So, } n_O^{\text{add}} = n_{\text{CO}_2}^r + n_{\text{H}_2\text{O}}^r \tag{3.43}$$

Calculations for $n_{\text{CO}_2}^r$ and $n_{\text{H}_2\text{O}}^r$ are given in appendix IV.

3.3.10 Ca - Balance

Ca enters the process from CaCO_3 and goes out in the form of CaO and CaS , i.e.

$$n_{\text{Ca}}^i = n_{\text{CaCO}_3} \quad (3.44)$$

(1 kg mole of CaCO_3 corresponds to 1 kg mole of Ca)

Also,

$$n_{\text{Ca}}^o = n_{\text{CaO}} + n_{\text{CaS}} \quad (3.45)$$

(1 kg mole both of CaO and CaS correspond to 1 kg mole of Ca each)

At steady state,

$$n_{\text{Ca}}^i = n_{\text{Ca}}^o \quad (3.46)$$

Combining equations (3.44) - (3.46), we get,

$$n_{\text{CaCO}_3} = n_{\text{CaO}} + n_{\text{CaS}} \quad (3.47)$$

3.3.11 Al_2O_3 Balance

Al_2O_3 enters the process from iron ore and ash of coal whereas it leaves in the slag i.e.

$$n_{\text{Al}_2\text{O}_3}^i = n_{\text{Al}_2\text{O}_3}^{\text{coal}} + n_{\text{Al}_2\text{O}_3}^{\text{ore}} \quad (3.48)$$

where

$$n_{\text{Al}_2\text{O}_3}^{\text{coal}} = \frac{C_x \left(\frac{\% \text{ ash}}{\text{in coal}} \right) \left(\frac{\% \text{ Al}_2\text{O}_3 \text{ in}}{\text{ash}} \right)}{102 \times 100 \times 100} \quad (3.49)$$

$$\text{Also, } n_{\text{Al}_2\text{O}_3}^o = n_{\text{Al}_2\text{O}_3} \quad (3.50)$$

$$\text{At steady state, } n_{\text{Al}_2\text{O}_3}^i = n_{\text{Al}_2\text{O}_3}^o \quad (3.51)$$

Combining equations (3.48) - (3.51), we get

$$n_{\text{Al}_2\text{O}_3}^{\text{ore}} = n_{\text{Al}_2\text{O}_3} - \frac{C_x \left(\frac{\% \text{ ash}}{\text{in coal}} \right) \left(\frac{\% \text{ Al}_2\text{O}_3 \text{ in}}{\text{ash}} \right)}{102 \times 100 \times 100} \quad (3.52)$$

3.4 HEAT BALANCE

The basic equation for the heat balance is:

$$\text{Heat supply} = \text{Heat Demand} + \text{Heat Accumulation} \quad (3.53a)$$

But for a process operating at steady state, there is no accumulation of heat. So, equation (3.53a) changes to

$$\text{Heat Supply} = \text{Heat Demand} \quad (3.53b)$$

3.4.1 Heat Demand

Here heat demands for melter - gasifier and reduction shaft furnace have been calculated separately. Finally these are combined to give the total heat demand for both the reactors i.e. melter gasifier and reduction shaft. All terms have been expressed in KJ/ kg mole of product Fe. Values used for enthalpy of formation and enthalpy increment equations are given in appendix I and II respectively.

3.4.1.1 Melter - Gasifier

The following metallurgical operations (each term in the is a metallurgical operation) are considered for calculating the heat demand in the melter-gasifier:

$$\begin{aligned} \left(\begin{array}{l} \text{Melter-gasifier} \\ \text{Heat Demand} \end{array} \right) &= \left(\begin{array}{l} \text{Hot Metal} \\ \text{Heat Demand} \end{array} \right) + \left(\begin{array}{l} \text{Slag} \\ \text{Heat Demand} \end{array} \right) \\ &+ \left(\begin{array}{l} \text{Heat Absorbed} \\ \text{by Endothermic} \\ \text{Reactions} \end{array} \right) + \left(\begin{array}{l} \text{Sensible Heat} \\ \text{of the Reduction} \\ \text{Gas leaving MG} \end{array} \right) + \\ &+ \left(\begin{array}{l} \text{Heat Demand} \\ \text{for Coal} \\ \text{Drying} \end{array} \right) + \left(\begin{array}{l} \text{Latent Heat of} \\ \text{Devolatilization} \\ \text{of Coal} \end{array} \right) + \left(\begin{array}{l} \text{Heat} \\ \text{Losses} \end{array} \right) \quad (3.54) \end{aligned}$$

(a) Hot Metal Heat Demand

Hot metal is considered to be tapped at T_M^O K. The amount of heat in hot metal at T_M^O K is the sensible heat and heat of mixing of various solute elements Fe, Mn, P and Fractions of Si and S coming from the reduction shaft furnace get heated up from 1200^O K

to T_M^O K whereas C and the rest S and Si coming from coal get heated up from 298K to T_M^O K.

(i) Heat required to raise the temperature of hot metal constituents to the tapping temperature (T_M^O K)

$$\begin{aligned}
 &= \left(44T_M - 40480 \right) n_{Fe(HM)} \\
 &+ \left(C/Fe \right) \left[23.5 T_M - 11800 \right] + n_{Si}^a \left[27.2 T_M + 17960 \right] \\
 &+ n_{Si}^c \left[27.2 T_M + 40400 \right] + \left(Mn/Fe \right) \left[48.6 T_M - 42640 \right] \\
 &+ n_S^a \left[18.7 T_M - 22440 \right] + n_S^c \left[18.7 T_M - 6250 \right] \\
 &+ \left(P/Fe \right) \left[18.65 T_M - 22380 \right] \quad (3.55)
 \end{aligned}$$

where $n_{Fe(HM)}$ i.e. kg moles of Fe in hot metal = 1. Calculation of n_{Si}^a , n_{Si}^c , n_S^a and n_S^c is given in appendix V.

(ii) Heat of mixing of C, Si, Mn, S and P in the hot metal

$$\begin{aligned}
 &= \left(C/Fe \right) \left(30000 \right) + \left(Si/Fe \right) \left(-95000 \right) \\
 &+ \left(Mn/Fe \right) \left(4000 \right) + \left(S/Fe \right) \left(-132384 \right) \\
 &+ \left(P/Fe \right) \left(-122640 \right) \quad (3.56)
 \end{aligned}$$

Adding equations (3.55) and (3.56), we get heat demand for the hot metal, i.e.

$$\begin{aligned}
 \left(\begin{array}{c} \text{Hot Metal} \\ \text{Heat Demand} \end{array} \right) &= \left(44 T_M - 40480 \right) + \left(C/Fe \right) \left(23.5 T_M + 18200 \right) \\
 &+ n_{Si}^a \left[27.2 T_M + 17960 \right] \\
 &+ n_{Si}^c \left[27.2 T_M + 40400 \right] + \left(Si/Fe \right) \left[-95000 \right] \\
 &+ \left(Mn/Fe \right) \left[48.6 T_M - 38640 \right] + n_S^a \left[18.7 T_M - 22440 \right] \\
 &+ n_S^c \left[18.7 T_M - 6250 \right] + \left(S/Fe \right) \left[-132384 \right] \\
 &+ \left(P/Fe \right) \left[18.65 T_M - 145020 \right] \quad (3.57)
 \end{aligned}$$

(b) Slag Heat Demand

Slag is also considered to be tapped at T_M^O K. The amount of heat in slag at T_M^O K is the sensible heat and heat of mixing.

CaO, MnO and fractions of SiO_2 , Al_2O_3 and S coming from reduction shaft furnace get heated up from 1200 K to T_M^O K whereas remaining SiO_2 , Al_2O_3 and S coming from coal get heated up from 298K to T_M^O K.

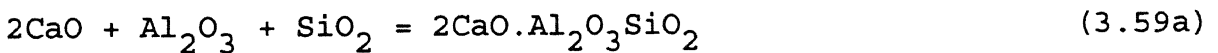
(i) Heat required to raise the temperature of the slag constituents to T_M^O K

$$\begin{aligned} &= n_{\text{CaO}} \left[55.5 \left(T_M - 1200 \right) \right] \\ &+ n_{\text{SiO}_2}^b \left[72.8 \left(T_M - 1200 \right) \right] + n_{\text{SiO}_2}^d \left[72.8 T_M - 26200 \right] \\ &+ n_{\text{Al}_2\text{O}_3}^{\text{ore}} \left[132 \left(T_M - 1200 \right) \right] + n_{\text{Al}_2\text{O}_3}^{\text{coal}} \left[132 T_M - 55000 \right] \\ &+ n_{\text{MnO}} \left[57.1 \left(T_M - 1200 \right) \right] + n_{\text{CaS}}^b \left[18.7 T_M - 22440 \right] \\ &+ n_{\text{CaS}}^d \left[18.7 T_M - 6250 \right] \end{aligned} \quad (3.58)$$

Values for $n_{\text{Al}_2\text{O}_3}^{\text{coal}}$ and $n_{\text{Al}_2\text{O}_3}^{\text{ore}}$ are taken from equations (3.49) and (3.52) respectively. Calculations for $n_{\text{SiO}_2}^b$, $n_{\text{SiO}_2}^d$, n_{CaS}^b and n_{CaS}^d are given in appendix V.

(ii) Heat of slag formation (d_{slag})

Following equations are considered in the slag formation:



Heat of slag formation is the heat released in slag formation per kg mole of product Fe.

$$d_{\text{slag}} = - \left[\left(n_{\text{CaO}} - n_{\text{Al}_2\text{O}_3} - n_{\text{SiO}_2} + n_{\text{MnO}} \right) .126840 \right. \\ \left. + \left(2 n_{\text{SiO}_2} - n_{\text{CaO}} - 2n_{\text{MnO}} \right) .90300 + n_{\text{Al}_2\text{O}_3} .104580 \right. \\ \left. + n_{\text{MnO}} . 24780 \right] \quad (3.60)$$

(d_{slag} has been calculated in the appendix VI)

Adding equations (3.58) and (3.60), we get heat demand for the slag, i.e.

$$\left(\begin{array}{c} \text{Slag Heat} \\ \text{Demand} \end{array} \right) = n_{\text{CaO}} \left[55.5 \left(T_M - 1200 \right) \right] \\ + n_{\text{SiO}_2}^b \left[72.8 \left(T_M - 1200 \right) \right] + n_{\text{SiO}_2}^d \left[72.8 T_M - 26200 \right] \\ + n_{\text{Al}_2\text{O}_3}^{\text{ore}} \left[132 \left(T_M - 1200 \right) \right] + n_{\text{Al}_2\text{O}_3}^{\text{coal}} \left[132 T_M - 55000 \right] \\ + n_{\text{MnO}} \left[57.1 \left(T_M - 1200 \right) \right] + n_{\text{CaS}}^b \left[18.7 T_M - 22440 \right] \\ + n_{\text{CaS}}^d \left[18.7 T_M - 6250 \right] + d_{\text{slag}} \quad (3.61)$$

(c) Heat Absorbed by Endothermic Reactions

Heat absorbing endothermic reactions occurring in the melter-gasifier are the reduction of oxides (namely, wustite, MnO, SiO_2 and P_2O_5 to Fe, Mn, Si and P respectively) and the decomposition of CaCO_3 .

The reactions are as follows:



$$\text{CaCO}_3 = \text{CaO} + \text{CO}_2 \quad (3.62e)$$

Fe, Mn, Si and P join hot metal whereas a part of CaO joins slag as it is and rest reacts with sulphur to form CaS which subsequently joins slag. The CO_2 component is transferred from solid CaCO_3 to the gas phase and hence it affects oxygen and carbon balances. Water gas reaction i.e. $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$ (3.62f) ($K=1$ at 821°C) [14] becomes less important from reduction of iron ore is rapidly reduced by C, i.e. $\text{C} + \text{H}_2\text{O} = \text{CO} + \text{H}_2$ (3.62g).

$$\text{Heat required for Wustite reduction} = n_{\text{Fe}_{0.95}\text{O}} \left(265000 \right) \quad (3.63)$$

$$\begin{aligned} \text{Heat required for SiO}_2 \text{ reduction} &= n_{\text{Si}}^a \left(\underset{\text{from ore}}{-H_{1200}^f} \right) + n_{\text{Si}}^c \left(\underset{\text{from coal}}{-H_{298}^f} \right) \\ &= n_{\text{Si}}^a \left(901000 \right) + n_{\text{Si}}^c \left(911000 \right) \end{aligned} \quad (3.64)$$

$$\begin{aligned} \text{Heat required for MnO reduction} &= \left(\text{Mn/Fe} \right) \left[\underset{\text{MnO}}{-H_{1200}^f} \right] \\ &= \left(\text{Mn/Fe} \right) \left(386000 \right) \end{aligned} \quad (3.65)$$

$$\begin{aligned} \text{Heat Required for P}_2\text{O}_5 &= 1/2 \left(\text{P/Fe} \right) \left(\underset{\text{P}_2\text{O}_5}{-H_{1200}^f} \right) \\ &= 1/2 \left(\text{P/Fe} \right) \left(1554000 \right) \end{aligned} \quad (3.66)$$

$$\text{Heat required for decomposition of CaCO}_3 = n_{\text{CaCO}_3} \left(561000 \right) \quad (3.67)$$

$$\begin{aligned} \text{Heat required for decomposition of H}_2\text{O} &= \frac{C_X \left(\% \text{ moisture in coal} \right)}{1800} \left(242000 \right) \end{aligned} \quad (3.68)$$

Adding (3.63) - (3.68), we get heat absorbed by endothermic reactions, ie.

$$\begin{aligned}
\left(\begin{array}{l} \text{Heat absorbed} \\ \text{by endothermic} \\ \text{reactions} \end{array} \right) &= n_{\text{Fe}_{0.95}\text{O}} \left(265000 \right) \\
&+ n_{\text{Si}}^{\text{a}} \left(901000 \right) + n_{\text{Si}}^{\text{c}} \left(911000 \right) + \left(\text{Mn/Fe} \right) \left(386000 \right) \\
&+ \left(\text{P/Fe} \right) \left(777000 \right) + n_{\text{CaCO}_3} \left(561000 \right) \\
&+ \frac{C_X \left(\% \text{ moisture in coal} \right)}{1800} \left(242000 \right) \quad (3.69)
\end{aligned}$$

Value for $n_{\text{Fe}_{0.95}\text{O}}$ is taken from equation (3.14).

(d) Sensible heat of the Reduction gas Leaving melter-gasifier

Reduction gas which consists of CO , H_2 , N_2 , CO_2 and H_2O leaves the melter-gasifier at a temperature T_R^{O} K. So, it carries away some sensible heat along with it which must be added to the heat demand.

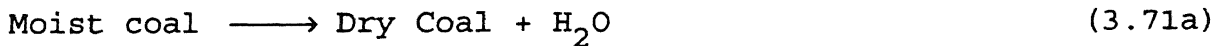
Sensible heat of the reduction gas exiting the MG (d_{rg})

$$\begin{aligned}
&= n_{\text{CO}}^{\text{r}} \left[34.2 T_R - 12600 \right] + n_{\text{H}_2}^{\text{r}} \left[30.9 T_R - 10300 \right] \\
&+ n_{\text{N}_2}^{\text{r}} \left[32.1 T_R - 10500 \right] + n_{\text{H}_2\text{O}}^{\text{r}} \left[43.7 T_R - 17900 \right] \\
&+ n_{\text{CO}_2}^{\text{r}} \left[56.3 T_R - 23100 \right] \quad (3.70)
\end{aligned}$$

(Calculations for n_{CO}^{r} , $n_{\text{H}_2}^{\text{r}}$, $n_{\text{N}_2}^{\text{r}}$, and $n_{\text{H}_2\text{O}}^{\text{r}}$ are given in appendix V)

(e) Heat demand for drying of coal

As the moist coal increases in temperature, water is the first constituent to evolve.



$$\text{Heat required for drying of coal} = \left(44000 \right) \frac{C_X \left(\% \text{ moisture in coal} \right)}{1800}$$

$$= 24.50 C_X \left(\% \text{ moisture in coal} \right) \quad (3.71b)$$

(f) Latent heat for Devolatilization of Coal

The latent heat of devolatilization is determined to be 626 KJ/kg (6). This also gets added to the melter-gasifier heat demand. As the temperature of coal increases devolatilization occurs according to the reaction :



$$\text{Latent Heat of Devolatilization} = 626.C_X \quad (3.73)$$

(g) Losses

Radiative and convective heat losses take place from melter-gasifier. In the absence of any data for above losses, we have taken losses as a variable term (Q_{MG}) in our model. Usually these losses are around 20000 KJ/kg mole of Fe

$$\text{Heat Losses} = Q_{MG} \quad (3.74)$$

Adding equations (3.57), (3.61), (3.69), (3.70) - (3.73), we get the heat demand for the melter-gasifier.

$$\begin{aligned} &\text{Melter-gasifier heat demand } (D_{MG}) \\ &= n_{\text{Fe}_{0.95}\text{O}} \left(265000 \right) + C_X \left[626 + 24.55 \left(\% \text{ moisture in coal} \right) \right] \\ &+ A \end{aligned} \quad (3.75)$$

where A denotes all other terms constituting the melter-gasifier heat demand. Substituting $n_{\text{Fe}_{0.95}\text{O}}$ from (3.14) in (3.72), we get

$$\begin{aligned} D_{MG} &= \left(100-X \right) \left(2789.47 \right) + C_X \left[626 + 24.50 \left(\% \text{ moisture in coal} \right) \right] \\ &+ A \end{aligned} \quad (3.76)$$

3.4.1.2 Reduction Shaft Furnace

$$\begin{aligned} \left(\begin{array}{l} \text{Reduction} \\ \text{shaft furnace} \\ \text{heat demand} \end{array} \right) &= \left(\begin{array}{l} \text{Heat demand for} \\ \text{heating iron ore} \\ \text{from 298K to 1200K} \end{array} \right) + \left(\begin{array}{l} \text{Heat demand} \\ \text{for iron ore} \\ \text{metallization} \end{array} \right) \\ &+ \left(\begin{array}{l} \text{Heat demand for} \\ \text{heating CaCO}_3 \\ \text{from 298 to 1200K} \end{array} \right) + \left(\begin{array}{l} \text{Sensible} \\ \text{heat of} \\ \text{top gas} \end{array} \right) + \left(\begin{array}{l} \text{Heat} \\ \text{Losses} \end{array} \right) \end{aligned} \quad (3.77)$$

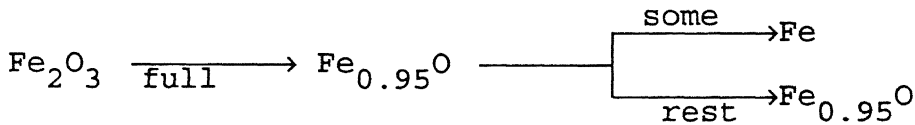
(a) Heat required for heating iron ore

It consists of heating of Fe_2O_3 , SiO_2 , MnO , Al_2O_3 , P_2O_5 , S from 298K to 1200K.

$$\begin{aligned}\text{Sensible heat of iron ore} &= \frac{1}{2} \left(129800 \right) + n_{\text{SiO}_2}^{\text{ore}} \left(61380 \right) \\ &+ \left[\left(\text{Mn/Fe} \right) + n_{\text{MnO}} \right] \left(46480 \right) + n_{\text{Al}_2\text{O}_3}^{\text{ore}} \left(103600 \right) \\ &+ \frac{1}{2} \left(\text{P/Fe} \right) \left(289600 \right) + n_{\text{FeS}}^{\text{ore}} \left(16170 \right)\end{aligned}\quad (3.78)$$

values for $n_{\text{SiO}_2}^{\text{ore}}$, $n_{\text{Al}_2\text{O}_3}^{\text{ore}}$ and $n_{\text{FeS}}^{\text{ore}}$ have been taken from equations (3.19), (3.52) and (3.27) respectively.

(b) Heat Demand for Iron ore Metallization



Heat demand for Fe_2O_3 reduction

$$\begin{aligned}\text{to Fe} &= n_{\text{Fe}} \frac{1}{2} \left(811000 \right) \\ &= n_{\text{Fe}} \left(405500 \right)\end{aligned}\quad (3.79)$$

Heat demand for Fe_2O_3 wustite reduction =

$$n_{\text{Fe}_{0.95}\text{O}} \left(120225 \right) \quad (3.80)$$

So, heat demand for iron ore metallization =

$$\left[n_{\text{Fe}} \left(405500 \right) + n_{\text{Fe}_{0.95}\text{O}} \left(120225 \right) \right] \quad (3.81)$$

Values for n_{Fe} and $n_{\text{Fe}_{0.95}\text{O}}$ have been taken from equations (3.13) and (3.14) respectively.

(c) Heat Demand for Heating CaCO_3

CaCO_3 gets heated up from 298K to 1200K in the reduction shaft furnace.

$$\text{Sensible heat} = n_{\text{CaCO}_3} (102600) \quad (3.82)$$

(d) Sensible Heat of Top Gas

Top gas which consists of CO, CO₂, H₂, H₂O and N₂ leave the reduction-shaft at T_g^o K. So, heat carried away by it (d_{tg}).

$$\begin{aligned} &= n_{\text{CO}}^{\text{tg}} [30.2 \text{ Tg} - 9100] + n_{\text{CO}_2}^{\text{tg}} [45.6 \text{ Tg} - 14100] \\ &\quad + n_{\text{H}_2}^{\text{tg}} [29.3 \text{ Tg} - 8800] + n_{\text{H}_2\text{O}}^{\text{tg}} [35.8 \text{ Tg} - 10800] \\ &\quad + n_{\text{N}_2}^{\text{tg}} [30.0 \text{ Tg} - 9000] \end{aligned} \quad (3.83)$$

(e) Heat Losses

Convective and radiative heat losses take place from reduction shaft furnace also. A variable Q_{RS} has been incorporated into the model for these losses.

$$\text{Reduction shaft losses} = Q_{\text{RS}} \quad (3.84)$$

Adding equations (3.78), (3.81) - (3.84), we get total heat demand for reduction shaft.

$$\begin{aligned} &\text{Heat demand for reduction shaft (D}_{\text{RS}}) \\ &= [n_{\text{Fe}} (405500) + n_{\text{Fe}_{0.95}\text{O}} (120225) + B] \end{aligned} \quad (3.85)$$

Where B denotes all other terms.

Substituting n_{Fe_{0.95}O} from (3.14) in (3.68), we get

$$D_{\text{RS}} = [(100 - X)1265.52 + B] + X(4055) \quad (3.86)$$

3.4.1.3 Two Stage Smelting Reduction Process

$$\begin{aligned} \left(\begin{array}{c} \text{Total} \\ \text{heat} \\ \text{demand} \end{array} \right) &= D_{\text{MG}} + D_{\text{RS}} - d_{\text{rg}} \\ &\quad + \left(\begin{array}{c} \text{Sensible heat loss during} \\ \text{cooling of the reduction} \\ \text{gas (d}_{\text{cooling}}) \end{array} \right) \\ &\quad + \left(\begin{array}{c} \text{Sensible heat loss during} \\ \text{taking out a portion of the} \\ \text{reduction gas from the process (d}_{\text{out}}) \end{array} \right) \end{aligned} \quad (3.87)$$

(a) Sensible heat loss during Cooling of the Reduction Gas

The reduction gas leaving the melter-gasifier at T_R^O K is cooled to T_C^O K before it enters the reduction shaft furnace. So, its sensible heat loss is given by

$$\begin{aligned} d_{\text{cooling}} = & \left(n_{\text{CO}}^r - n_{\text{CO}}^{\text{ro}} \right) \left[34.2 \left(T_R - T_C \right) \right] \\ & + \left(n_{\text{CO}_2}^r - n_{\text{CO}_2}^{\text{ro}} \right) \left[56.3 \left(T_R - T_C \right) \right] \\ & + \left(n_{\text{H}_2\text{O}}^r - n_{\text{H}_2\text{O}}^{\text{ro}} \right) \left[43.7 \left(T_R - T_C \right) \right] \\ & + \left(n_{\text{H}_2}^r - n_{\text{H}_2}^{\text{ro}} \right) \left[30.9 \left(T_R - T_C \right) \right] \\ & + \left(n_{\text{N}_2}^r - n_{\text{N}_2}^{\text{ro}} \right) \left[32.1 \left(T_R - T_C \right) \right] \end{aligned} \quad (3.88)$$

(b) Sensible Heat Loss in Surplus Reduction gas

In case, when the reduction gas is more than required, the difference (produced-required) is taken out of the process and is termed as surplus gas. So, sensible heat taken by surplus gas must be added to the total heat demand of the process.

$$\begin{aligned} d_{\text{out}} = & n_{\text{CO}}^{\text{ro}} \left[34.2 T_R - 12600 \right] \\ & + n_{\text{CO}_2}^{\text{ro}} \left[56.3 T_R - 23100 \right] \\ & + n_{\text{H}_2}^{\text{ro}} \left[30.9 T_R - 10300 \right] \\ & + n_{\text{H}_2\text{O}}^{\text{ro}} \left[43.7 T_R - 17900 \right] \\ & + n_{\text{N}_2}^{\text{ro}} \left[32.1 T_R - 10500 \right] \end{aligned} \quad (3.89)$$

Calculations for $n_{\text{CO}}^{\text{ro}}$, $n_{\text{CO}_2}^{\text{ro}}$, $n_{\text{H}_2}^{\text{ro}}$, $n_{\text{H}_2\text{O}}^{\text{ro}}$ and $n_{\text{N}_2}^{\text{ro}}$ have been shown in the appendix IV.

Adding equations (3.76), (3.86), (3.88) and (3.89) and subtracting (3.70), we get total heat demand for the overall process, i.e.

Total heat demand for the process (D_{total}) =

$$\left\{ \left[(100 - X) 2789.47 \right] + C_X \left[626 + 24.50 \left(\% \text{ moisture in coal} \right) \right] \right. \\ \left. + A \right\} + \left[(100 - X) 1265.52 + X (4055) + B \right] \\ + d_{\text{out}} + d_{\text{cooling}} - d_{\text{rg}} \quad (3.90)$$

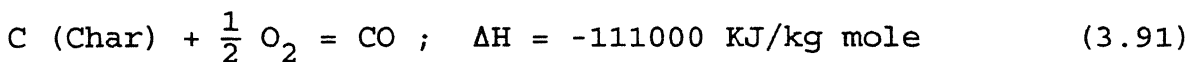
3.4.2 Heat Supply

In the two stage smelting reduction process necessary heat can be supplied by the following possible ways.

3.4.2.1 Combustion of Coal

The combustion of coal occurs in the melter-gasifier with the help of pure oxygen. In the melting zone the furnace gases are at thermal and chemical equilibrium with the molten metal which is around 1700 - 1850 K with a relatively high carbon content. Therefore the combustion of coal will result in the formation of carbon monoxide and hydrogen. Typical coal composition of different ranks is given in appendix VII.

The following reaction occurs when coal combusts in the melter-gasifier:

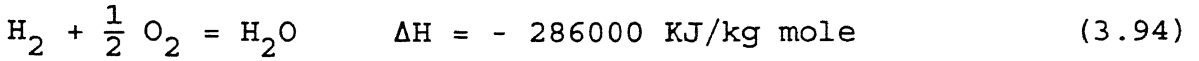
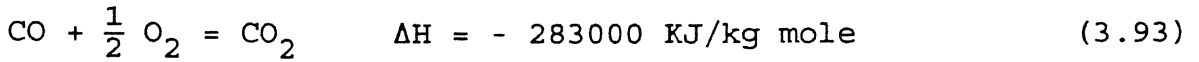


$$\text{Heat supplied by combustion of coal } (S_{\text{coal}}) = n_C^A (111000) \quad (3.92)$$

3.4.2.2 Post-combustion of Reducing Gas

The reducing gas consists of CO and H₂. Both gases have high calorific value. Their combustion in the MG results in saving of coal. Secondary oxygen from top has to be supplied to combust a portion of the CO and H₂ above the bath to provide greater heat liberation. Post combustion of CO and H₂ to CO₂ and H₂O respectively results in the transfer of the heat thus produced to

the hot metal bath according to the following reactions.



The necessary amount of oxygen is to be supplied from top of the melter-gasifier.

Degree of post combustion is defined by [12] :

$$(\text{ppc}) = \frac{\left(\% \text{CO}_2 + \% \text{H}_2\text{O} \right) \times 100}{\left(\% \text{CO} + \% \text{CO}_2 + \% \text{H}_2 + \% \text{H}_2\text{O} \right)} \quad (3.95)$$

The necessary O_2 is supplied from top for post-combustion. The transfer of heat occurs via slag to metal bath. Now, Fractional heat transfer to bath [3] (α) =

$$\frac{\text{Heat supplied to bath}}{\text{Heat produced by post-combustion}} \times 100 \quad (3.96)$$

It is assumed that $\alpha = 100\%$

Heat supplied by post-combustion (S_{PC})

$$= \left[283000 n_{\text{CO}_2}^r + 286000 n_{\text{H}_2\text{O}}^r \right] \quad (3.97)$$

Calculations for $n_{\text{CO}_2}^r$ and $n_{\text{H}_2\text{O}}^r$ have been shown in appendix

IV.

From the above it follows that

Total heat supply (S_{total}) = $S_{\text{coal}} + S_{\text{PC}}$ =

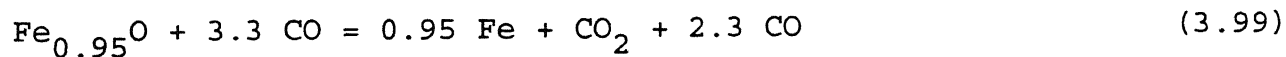
$$\left[n_{\text{C}}^A (111000) + n_{\text{CO}_2}^r (283000) + n_{\text{H}_2\text{O}}^r (286000) \right] \quad (3.98)$$

3.4.3 Output of the Model

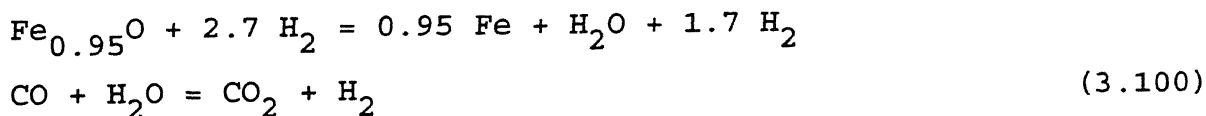
3.4.3.1 (CO+H₂) requirement for the reduction in the reduction shaft furnace

The reduction gas exiting the melter gasifier is circulated completely or partially in the reduction shaft furnace. Depending on its amount varying degree of metallization can be achieved. Therefore, (CO+H₂) requirement has been calculated as a function of degree of metallization.

From Fe-O-C and Fe-O-H equilibrium curves, it is clear that at 1200 K the equilibrium concentration of CO for Fe₃O₄ - Wustite is 20% whereas that for wustite to Fe about 70% i.e. the extent of utilisation of CO = (%CO₂ x 100)/(% CO + %CO₂) is at a maximum of 80% in respect of magnetite/wustite equilibrium and only 30% for wustite/iron equilibrium. i.e.



After reduction of wustite at 30% utilisation, CO-CO₂ gas mixture will have sufficient reduction potential for removal of rest of oxygen from magnetite and haematite. Hydrogen is also a very active reducing agent. In case of wustite reduction by hydrogen at 1200K maximum utilisation is 37% i.e.



It is clear from equation (3.99) and (3.100) that 1 kg mole of H₂ will replace 1.22 kg moles of CO as far as their mutual reduction efficiency of wustite is concerned at 1200K. Considering above facts final equation for reduction of Fe_{0.95}O to Fe by a mixture of CO and H₂ takes following form:

$$\begin{aligned}
& \text{Fe}_{0.95}\text{O} + (3.3 - 1.22 n_{\text{H}_2}^r) \text{CO} + (n_{\text{H}_2}^r) \text{H}_2 \\
& = 0.95 \text{Fe} + \frac{(3.3 - 1.22 n_{\text{H}_2}^r)}{3.3} \text{CO}_2 \\
& + \frac{2.3}{3.3} (3.3 - 1.22 n_{\text{H}_2}^r) \text{CO} + \left(\frac{n_{\text{H}_2}^r}{2.7} \right) \text{H}_2\text{O} \\
& + \left(\frac{1.7}{2.7} \right) n_{\text{H}_2}^r \text{H}_2 \quad (3.101)
\end{aligned}$$

If $n_{\text{H}_2}^r = 2.7$, then equation (3.101) reduces to (3.100) whereas if $n_{\text{H}_2}^r = 0$, then equation reduces to (3.99). H_2 replacement occurs in the range $0 < n_{\text{H}_2}^r < 2.7$.

Now $(\text{CO} + \text{H}_2)$ generated by reaction (3.101) (which is considered to be the most difficult step in haematite to iron reduction) should be sufficient enough to take care of haematite to magnetite and magnetite to wustite reduction, otherwise iron will not form. Calculation of the point upto which thermodynamic requirement of iron formation gets fulfilled :

We know that to make iron, 428.5 kg and 300.7 kg oxygen has to be removed per 1000 kg Fe from Fe_2O_3 and $\text{Fe}_{0.95}\text{O}$ respectively. So, if Y kg oxygen is removed from smelting reduction stage then remaining $(428.5 - Y)$ kg oxygen will be removed in pre-reduction stage out of which $(300.7 - Y)$ kg is removed in the most difficult stage of $\text{Fe}_{0.95}\text{O}$ to Fe reduction.

Direct reduction of pre-reduced ore in smelting - reduction stage -



$$\text{CO produced (For removing Y kg oxygen)} = 28Y/16 \text{ kg} \quad (3.103)$$

Indirect reduction of iron ore in pre-reduction stage - (See

reaction (3.101)

CO required (For removing (300.7-Y) kg oxygen)

$$= \frac{\left(3.3 - 1.22 n_{H_2}^r\right) \times 28 (300.7 - Y)}{16} \quad (3.104)$$

Equating CO produced generated, we get,

$$\Rightarrow \frac{28Y}{16} = \frac{\left(3.3 - 1.22 n_{H_2}^r\right) \times 28 (300.7 - Y)}{16} \quad (3.105)$$

So, reduction in smelting reduction stage (direct reduction)

$$\begin{aligned} R &= \frac{\text{Oxygen removed in this stage}}{\text{Total oxygen to be removed}} \times 100 \\ &= \frac{300.7 \left(3.3 - 1.22 n_{H_2}^r\right)}{428.5 \left(4.3 - 1.22 n_{H_2}^r\right)} \\ &= \frac{0.702 \left(3.3 - 1.22 n_{H_2}^r\right)}{\left(4.3 - 1.22 n_{H_2}^r\right)} \quad (3.106) \end{aligned}$$

$$\text{So, \% pre-reduction (T)} = (100 - R) \quad (3.107)$$

Therefore, calculations performed for (CO+H₂) requirement are valid for B% pre-reduction or more.

Relating O/Fe and % pre-reduction, we get

$$O/Fe = (150 - 1.5T)/100 \quad (3.108)$$

$$\text{Also } O/Fe = \frac{b}{a + 0.95b} = b \quad (3.109)$$

(Our basis being 1 kg mole Fe $a + 0.95b = 1$)

$$a = (1 - 0.95b)$$

% Metallization upto which our calculations are valid

$$\begin{aligned} &= \frac{a \times 100}{a + 0.95b} \\ &= 100 a \\ &= 100 (1 - 0.95b) \\ &= 100 \left[1 - 0.95 \left(\frac{150 - 1.5T}{100}\right)\right] \quad (3.110) \end{aligned}$$

(CO+H₂) requirement for production of 1 kg mole of Fe from

equation (3.101) i.e. when 100% metallization is there

$$= \frac{\left[\left\{ 3.3 - 1.22 \left(n_{H_2}^r \right)'' \right\} + \left(n_{H_2}^r \right)'' \right]}{0.95} \quad (3.111)$$

So, $(CO+H_2)$ requirement for X% metallization

$$= \left(\frac{X}{100} \right) \frac{\left[\left\{ 3.3 - 1.22 \left(n_{H_2}^r \right)'' \right\} + \left(n_{H_2}^r \right)'' \right]}{0.95} \quad (3.112)$$

By equating heat demand and supply, the following are calculated :

3.4.3.2 $(CO+H_2)$ production in the Melter Gasifier

(a) *When only Melter gasifier thermal and chemical demand is met by coal combustion*

Here calculations are made by considering that the two-stage smelting reduction is performed by controlling the thermal and chemical demand of the melter-gasifier only. The reduction gas existing melter gasifier is circulated completely or partially in the reduction shaft furnace and depending on its amount varying degree of metallization can be achieved.

Here $(CO+H_2)$ produced has been calculated in terms of X (the degree of metallization). Now at X% metallization, we know that

$$n_{Fe} = \frac{X}{100} \quad (3.13)$$

$$n_{Fe_{0.95}O} = \left(\frac{100 - X}{95} \right) \quad (3.14)$$

So, at any metallization we will have a mixture of Fe and $Fe_{0.95}O$ from reduction shaft furnace.

Heat balance for melter - gasifier becomes :

$$D_{MG} = S_{total} \quad (3.113)$$

Using equations (3.76) and (3.98) for D_{MG} and S_{total} respectively, we get

$$\begin{aligned} & \left[(100 - X) 2789.47 + C_X \left[626 + 24.50 (\% \text{ moisture in coal}) \right] \right] + A \\ & = \left[n_C^A (111000) + n_{CO_2}^r (283000) + n_{H_2O}^r (286000) \right] \end{aligned} \quad (3.114)$$

Here A = Other terms constituting heat demand for melter-gasifier (a constant)

When no metallization is done i.e. $X = 0$, we get only $Fe_{0.95}O$ from reduction shaft furnace. Then from equation (3.76), we have Melter gasifier heat demand for no metallization, i.e. at $X = 0$

$$\begin{aligned} D_{MGO} &= (2789.47) (100) + C_0 [626 + 24.50 (\% \text{ moisture in coal})] \\ &+ A \end{aligned} \quad (3.115)$$

Here C_0 = kg coal for 0% metallization per kg mole of product iron
Carrying out the heat balance for melter-gasifier, equation (3.114) modifies to

$$\begin{aligned} & [(100) (2789.47) + C_0 [626 + 24.50 (\% \text{ moisture in coal})] + A \\ & = [n_C^{A'} (111000) + n_{CO_2}^{r'} (283000) + n_{H_2O}^{r'} (286000)] \end{aligned} \quad (3.116)$$

Here $n_C^{A'}$, $n_{CO_2}^{r'}$ and $n_{H_2O}^{r'}$ are corresponding values of n_C^A , $n_{CO_2}^r$ and $n_{H_2O}^r$ respectively at $C_X = C_0$. In above equation, C_0 being the only unknown, can be calculated.

Now for $\left(\frac{(100-X)}{95} \right)$ kg moles of $Fe_{0.95}O$ coal requirement in kg coal/kg mole of product Fe = $\left(\frac{100-X}{95} \frac{C_0}{1.05} \right)$

So, corresponding CO and H_2 in the reduction gas can be calculated in terms of X (see appendix IV).

$$\begin{aligned} \left(n_{CO}^r \right)_{wus} &= \left[\left(\frac{100 - X}{95 \times 1.05} \right) \frac{C_0 (\% \text{ C in coal})}{1200} + n_{CaCO_3} - C/Fe \right] \\ & \left(1 - \frac{ppc}{100} \right) \end{aligned} \quad (3.117)$$

$$\begin{aligned} \left(n_{H_2}^r \right)_{wus} &= \left(\frac{100 - X}{95 \times 1.05} \right) C_0 \left[\frac{(\% \text{ H in coal})}{200} + \frac{(\% \text{ moisture in coal})}{1800} \right] \\ & \left(1 - \frac{ppc}{100} \right) \end{aligned} \quad (3.118)$$

Now when 100% metallization is done

i.e. $X = 100$, we get complete Fe from reduction shaft furnace.

Then from equation (3.76), we have

Melter gasifier heat demand for 100% metallization

$$(X = 100), D_{MG,100} = C_{100} \left[626 + 24.50 \left(\% \text{ moisture in coal} \right) \right] + A \quad (3.119)$$

Here C_{100} = kg coal for 100% metallization per kg mole of product Fe.

Carrying out the heat balance for melter gasifier, equation (3.114) modifies to

$$C_{100} \left[626 + 24.5 \left(\% \text{ moisture in coal} \right) \right] + A = \left[n_C^A \left(111000 \right) + n_{CO_2}^r \left(283000 \right) + n_{H_2O}^r \left(28600 \right) \right] \quad (3.120)$$

Here n_C^A , $n_{CO_2}^r$ and $n_{H_2O}^r$ are corresponding values of n_C^A , $n_{CO_2}^r$ and $n_{H_2O}^r$ respectively at $C_X = C_{100}$.

In above equation C_{100} is the only unknown, so it can be calculated.

Now for $(X/100)$ kg moles of Fe, coal requirement in kg coal/kg mole of product iron - $(X/100)C_{100}$. So, corresponding CO and H_2 can be calculated in terms of X (see appendix IV).

$$\left(n_{CO}^r \right)_{Fe} = \left[\left(\frac{X}{100} \right) \frac{C_{100} (\%C \text{ in coal})}{1200} + n_{CaCO_3} - C/Fe \right] \left(1 - \frac{ppc}{100} \right) \quad (3.121)$$

$$\left(n_{H_2}^r \right)_{Fe} = \left(\frac{X}{100} \right) C_{100} \left[\frac{\%H \text{ in Coal}}{200} + \frac{\% \text{ moisture in coal}}{1800} \right] \left(1 - \frac{ppc}{100} \right) \quad (3.122)$$

Now total production of $(CO + H_2)$ is the sum of (3.117), (3.118), (3.121) and (3.122) i.e.

$$\begin{aligned}
(\text{CO} + \text{H}_2) \text{ production} &= \left(n_{\text{CO}}^r \right)_{\text{wus}} + \left(n_{\text{CO}}^r \right)_{\text{Fe}} + \left(n_{\text{CO}_2}^r \right)_{\text{wus}} + \left(n_{\text{H}_2}^r \right)_{\text{Fe}} \\
&= \left(n_{\text{CO}}^r \right)_t + \left(n_{\text{H}_2}^r \right)_t \\
&= \left(1 - \frac{\text{ppc}}{100} \right) \left\{ \left[\left(\frac{100 - X}{95 \times 1.05} \right) \frac{C_O (\% \text{C in Coal})}{1200} + \left(\frac{X}{100} \right) \frac{C_{100} (\% \text{C in Coal})}{1200} \right] \right. \\
&\quad \left. + 2 \left[n_{\text{CaCO}_3} - C/\text{Fe} \right] + \left[\left(\frac{100 - X}{95 \times 1.05} \right) C_O + \left(\frac{X}{100} \right) C_{100} \right] \right. \\
&\quad \left. \left[\frac{(\% \text{H in Coal})}{200} + \frac{\% \text{moisture in Coal}}{1800} \right] \right\} \quad (3.123)
\end{aligned}$$

(b) *When thermal and chemical demand for the both reactors is met by coal combustion*

Here the way of calculation remains to be the same as for previous case where only the melter-gasifier thermal and chemical demand is considered. The only difference will be in the heat demand terms due to which equation (3.115) for heat demand at 0% metallization will change to :

$$\begin{aligned}
&\text{overall heat demand for no metallization (X= 0), } D_{\text{total}, 0} \\
&= \{ [(100)(2789.47)] + C_0 [626 + 24.50 (\% \text{ moisture in coal}) + A] \\
&\quad + [(100)(1265.52) + X(4055) + B] + d_{\text{out}} + d_{\text{cooling}} - d_{\text{rg}} \} \quad (3.124)
\end{aligned}$$

$$\begin{aligned}
&\text{overall heat demand for 100\% metallization (X = 100), } D_{\text{total}, 100} \\
&= \{ C_{100} [626 + 24.50 (\% \text{ moisture in coal})] \} + A + B + 405500 \\
&\quad + d_{\text{out}} + d_{\text{cooling}} - d_{\text{rg}} \quad (3.125)
\end{aligned}$$

Rest all procedure for the calculation of $(\text{CO} + \text{H}_2)$ production is the same as done before.

3.4.3.3 Surplus Reduction Gas

The surplus reduction gas is calculated by considering production and requirement. The reduction gas in the reduction

shaft furnace is required to perform reduction of iron oxides to Fe and $\text{Fe}_{0.95}\text{O}$. For 100% metallization in the reduction shaft furnace, the amount of reduction gas requirement is very high as compared to 0% metallization where amount of reduction gas requirement is low. So, the amount of surplus reduction gas is calculated from:

$$\text{Surplus reduction gas} = \text{Production} - \text{requirement} \quad (3.126a)$$

The surplus energy (KJ) is calculated by equation :

$$\text{Surplus energy} = \left[\begin{array}{l} \text{Kg moles} \\ \text{of CO in} \\ \text{surplus gas} \end{array} \right] 283000 + \left[\begin{array}{l} \text{Kg moles} \\ \text{of H}_2 \text{ in} \\ \text{surplus gas} \end{array} \right] 286000 \quad (3.126b)$$

3.4.3.4 Coal rate, Oxygen requirement for Coal Combustion and Post combustion, Reduction gas and Top gas Amount and Composition

(a) *When only the melter-gasifier thermal and chemical demand is met by coal combustion*

Heat balance for melter - gasifier is given by

$$\begin{aligned} & \left[(100 - X) 2789.47 + C_X \left[626 + 24.50 (\% \text{ moisture in coal}) \right] \right] + A \\ & = \left[n_C^A (111000) + n_{\text{CO}_2}^r (283000) + n_{\text{H}_2\text{O}}^r (286000) \right] \end{aligned} \quad (3.114)$$

Here A = Other terms constituting heat demand for melter-gasifier (a constant)

Now

$$n_{\text{CO}_2}^r = n_C^A \frac{\text{ppc}}{100} \quad (3.127)$$

$$n_{\text{H}_2\text{O}}^r = n_{\text{H}_2}^o \frac{\text{ppc}}{100} = \frac{n_{\text{H}}^o}{2} \frac{\text{ppc}}{100} \quad (3.128)$$

(Both taken from appendix IV)

Substituting n_C^A and n_{H}^o from (3.9) and (3.32) in above equations, we get

$$n_{\text{CO}_2}^r = \left[\frac{C_X (\% \text{ C in coal})}{1200} + n_{\text{CaCO}_3} - \left[\text{C/Fe} \right] \right] \frac{\text{ppc}}{100} \quad (3.129)$$

$$n_{H_2O}^r = \left[\frac{C_X (\% \text{ H in coal})}{200} + \frac{C_X (\% \text{ moisture in coal})}{1800} \right] \frac{ppc}{100} \quad (3.130)$$

Substituting $n_{CO_2}^r$, $n_{H_2O}^r$ and n_C^A in equation (3.114) from (3.129), (3.130) and (3.9), we get an equation which contains two unknowns, viz, X (degree of metallization) and C_X (kg coal/kg mole of product Fe). So, if we specify % metallization, we can get information about coal rate (i.e. C_X can be calculated).

i.e. Coal requirement for X% metallization (kg/thm)

$$\begin{aligned} &= C_X \frac{1000}{56} \frac{(\% \text{ Fe in hot metal})}{100} \\ &= \frac{C_X (\% \text{ Fe in hot metal})}{5.6} \end{aligned} \quad (3.131)$$

Substituting C_X in equations for n_{CO}^r , $n_{CO_2}^r$, $n_{H_2}^r$ and $n_{N_2}^r$ (given in the appendix IV), we get composition amount of the reduction gas.

Also amounts of various gas components can be determined in Nm^3 /thm.

$$\begin{aligned} \text{CO in reduction gas (Nm}^3\text{/thm)} &= n_{CO}^r (22.4) \frac{1000}{56} \frac{(\% \text{ Fe in hot metal})}{100} \\ &= \frac{n_{CO}^r (22.4) (\% \text{ Fe in HM})}{5.6} \end{aligned} \quad (3.132)$$

Similarly, CO_2 , H_2 , H_2O and N_2 in reduction gas leaving melter gasifier can be calculated. Reduction gas thus produced is circulated to the RSF where it carries out reduction of iron ore. Top gas calculations are made considering the reduction requirement in the RSF.

Substituting C_X in equations for n_{CO}^{tg} , $n_{CO_2}^{tg}$, $n_{H_2}^{tg}$, $n_{H_2O}^{tg}$ and $n_{N_2}^{tg}$ (given in the appendix IV), we get composition and amount of the top gas.

Amounts of various gas components can be determined in Nm^3 /thm.

$$\text{CO in top gas (Nm}^3\text{)} = n_{CO}^{tg} (22.4) \frac{1000}{56} \frac{(\% \text{ Fe in hot metal})}{100}$$

$$= \frac{n_{CO}^U (22.4) (\% \text{ Fe in HM})}{5.6} \quad (3.133)$$

Similarly, CO_2 , H_2 , H_2O and N_2 in the top gas can be calculated.

$n_{CO_2}^r$ and $n_{H_2O}^r$ being known now, secondary oxygen requirement for post-combustion (Nm^3/thm) can be calculated.

Secondary oxygen requirement (Nm^3/thm) =

$$\left(\frac{n_{H_2O}^r}{2} + \frac{n_{CO_2}^r}{2} \right) \frac{22.4 (\% \text{ Fe in HM})}{5.6} \quad (3.134)$$

Now from oxygen balance i.e. equation (3.42), n_O^B can be calculated.

So oxygen requirement for coal combustion =

$$\frac{n_O^B}{2} \times \frac{22.4 (\% \text{ Fe in hot metal})}{5.6} \quad (3.135)$$

(b) When thermal and chemical demands of both the reactors are met by coal combustion

Heat balance for overall process becomes:

$$D_{total} = S_{total} \quad (3.136)$$

Using equations (3.90) and (3.98) for D_{total} and S_{total} respectively, we get

$$\begin{aligned} & \{ \{100 - X\} 2789.47 \} + C_X \{ \{626 + 24.50 (\% \text{ moisture in coal}) \} + A \} \\ & + A \} + \{ (100 - X) 1265.52 + B \} + X(4055) \} + d_{out} \\ & + d_{cooling} - d_{rg} = \\ & [n_C^A (111000) + n_{CO_2}^r (283000) + n_{H_2O}^r (286000)] \end{aligned} \quad (3.137)$$

(Here A and B are constant heat demand terms)

Rest all procedure to calculate coal rate, oxygen requirements, gas amount and composition is the same as done for previous case when only the melter-gasifier heat demand was considered.

3.5 METHOD OF CALCULATION

For the thermo-chemical model developed in previous sections of this chapter, a computer program in FORTRAN 77 has been made. Flow-chart of the computer program is shown in Figure 3.2. All calculations have been performed in HP-9000 series which operates on UNIX environment. The basis of calculation is 1 kg mole of Fe. For the sake of calculations, the following values are taken:

HM Composition

% C = 4.06 %Si = 0.39 %Mn = 0.6 %S = 0.109 %P = 0.152

Slag Composition

%CaO = 37 %SiO₂ = 31 %MnO = 10 %Al₂O₃ = 20 %CaS = 2

Basicity of slag (%CaO/%SiO₂) \approx 1.2

This basicity is normally maintained in the COREX process.

Ash Composition

%SiO₂ = 61.66 %Al₂O₃ = 38.34

Hot Metal Temperature 1527°C

Temperature of the reduction gas leaving MG 1000°C

(No cooling of the reduction gas is considered)

Losses 20000 KJ/kg mole of Fe

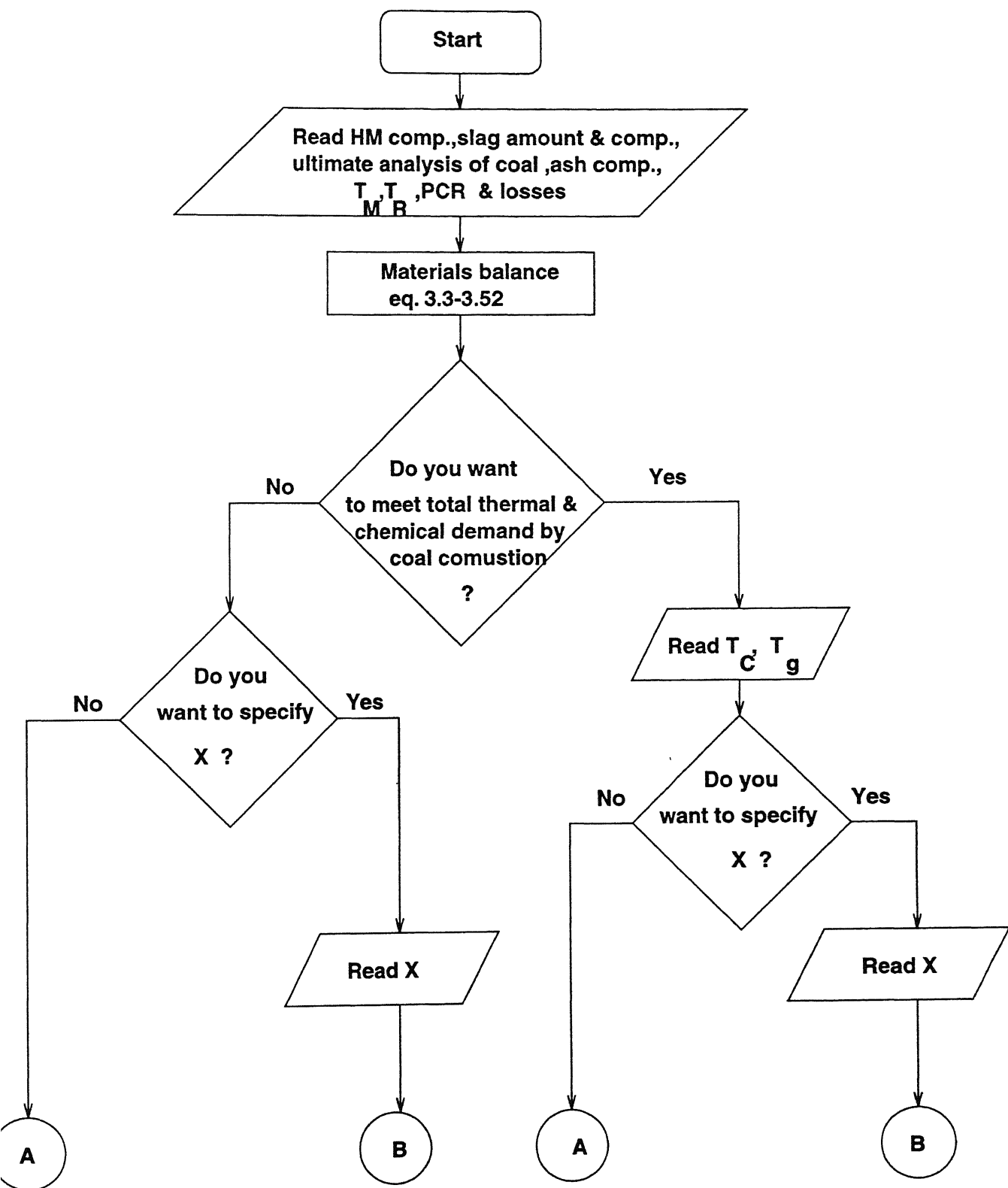
Top Gas Temperature 200°C

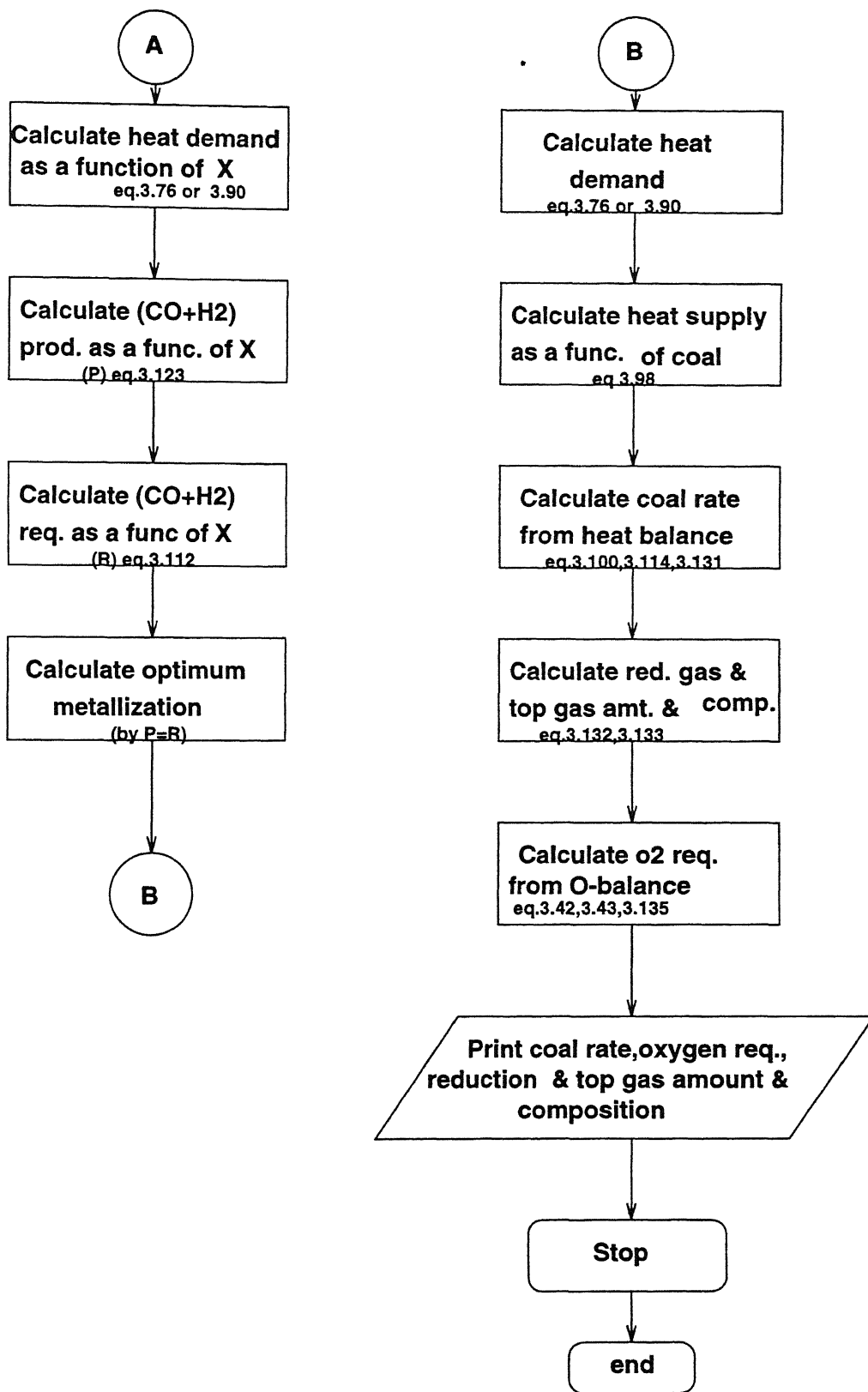
For calculations it has been assumed that S from ore joins the hot metal and slag in the same ratio as the S from coal. Similar assumption has been taken for Si too.

Effect of the following variables can be seen on coal rate, oxygen requirements, reduction gas and top gas amount and composition and the optimum metallization :

Degree of metallization (0 - 100%)

Degree of post-comb. (0 - 50%)





**Fig 3.2 : FLOW CHART OF THE COMPUTER PROGRAM FOR THE MODEL
FOR TWO-STAGE SMELTING REDUCTION PROCESS**

Slag amount

(350 - 550) Kg/thm

Coal rank

Sub-bituminous, bituminous and anthracite

(Their composition is given in the appendix VII)

3.6 Model Verification

In order to verify the model calculations, comparisons have been made between the plant data on coal consumption with that of the model values for identical set of input variables. This comparison can be seen in Table 3.1 and is plotted in Fig. 3.3. The plant data is given for consumption of the coal of the following composition:

% Ash = 16.24 % VM = 27.43 % Fixed Carbon = 56.3

% C = 80.59 %H = 4.86 % O = 12.33 % N = 1.81

%P = 0.015 %S = 0.87

The Fig. 3.3 and te Table 3.1 show that the predicted values of coal are around 81-86% of the actual values for different slag rates and hot metal composition. This differences may be attributed to the following reasons:

- 1) In the COREX process, fluidized bed for combustion of coal particles is employed. Loss of carbon in the dust also occurs. The actual plant data does not give the percentage loss of carbon in the dust. According to some estimate this loss of carbon in dust comes around 10% of the coal rate [19]. In the absence of this data the model will calculate the value of the coal consumption lower than the actual.
- 2) An increase in radiative and convective heat losses by 5% amounts to an incrase in coal rate by 0.95%. In the model we have assumed losses (radiative and convective) to be 20000

Table 3.1 : Comparison of Plant Data with Model Values

C %	Si %	S %	P %	Temp. (°C)	Slag rate kg/thm	Coal rate kg/thm	Predicted coal rate kg/thm
3.8	1.25	.119	.115	1479	346	1169	985
3.66	0.91	.127	.125	1481	423	1227	1042
3.84	0.93	.113	.117	1483	417	1250	1052
4.06	0.39	.109	.182	1475	450	1221	1042
4.28	0.38	.083	.176	1469	410	1107	932
4.26	0.32	.084	.158	1464	440	1177	1012
4.17	0.48	.076	.170	1465	420	1345	1117
4.10	0.40	.072	.130	1462	430	1146	978
4.21	0.32	.065	.170	1465	440	1118	951
4.18	0.31	.065	.140	1465	400	1090	903
4.27	0.60	.064	.140	1464	470	1238	1025
3.92	0.54	.100	.140	1427	460	1097	932
4.16	0.31	.078	.200	1457	539	1186	1003
4.43	0.29	.060	.173	1462	515	1105	931
4.00	0.70	.130	.130	1417	500	1067	896
4.36	0.33	.046	.156	1461	504	1131	962
4.30	0.27	.062	.146	1456	554	1245	1012

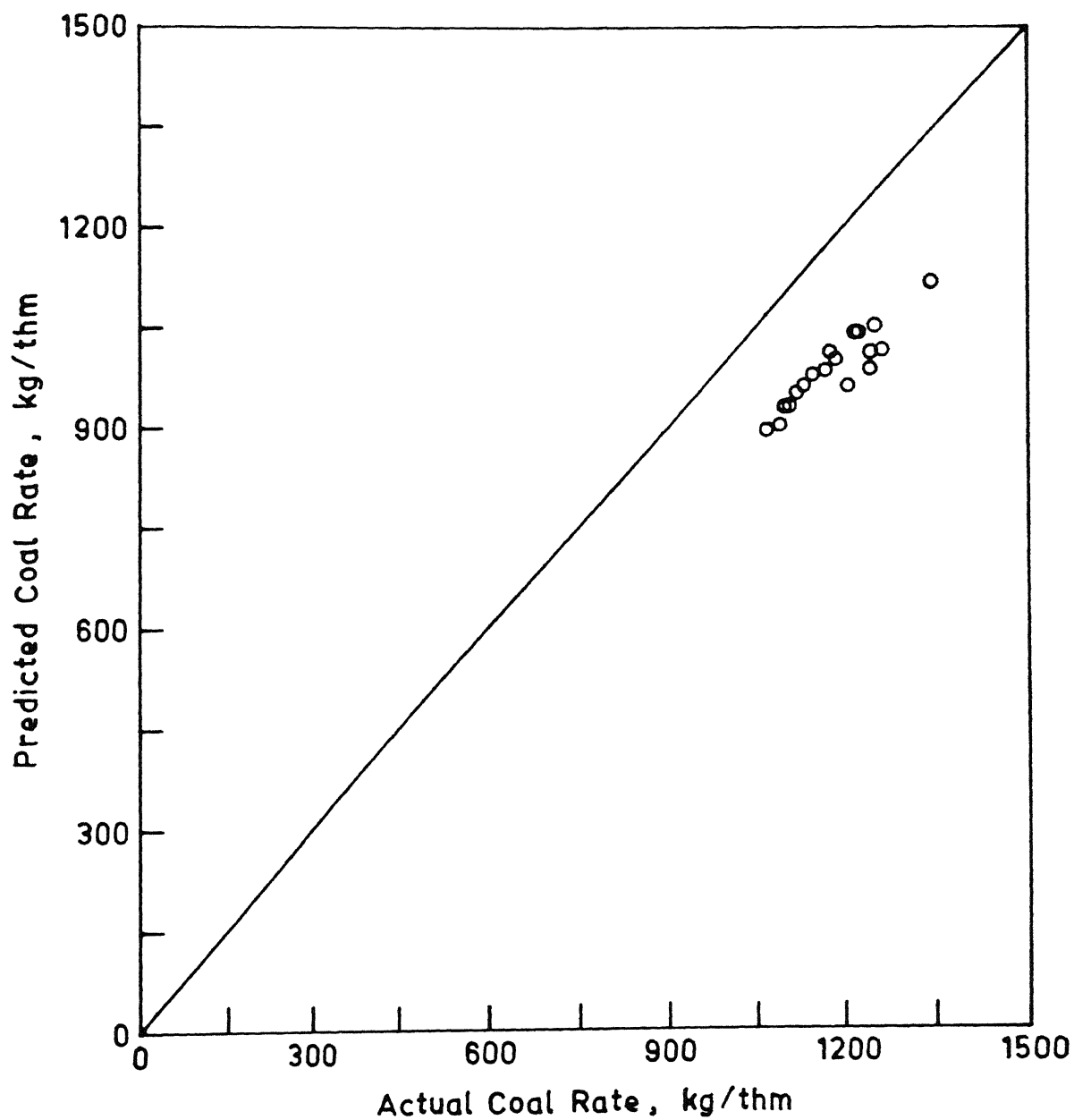


Fig. 3.3 Predicted coal rate vs. actual coal rate

KJ/kg mole of Fe (around 2.5% of the total thermal and chemical demand). Due to lack of data on radiative and convective heat losses, some error gets introduced in the predicted values.

In the light of above arguments, we can say that the difference between model predictions and the actual values is justified. If data about the heat and dust losses are available, our model can make predictions with very good accuracy.

CHAPTER - 4

RESULTS AND DISCUSSIONS

The thermochemical model results (coal consumption, oxygen requirements, reduction gas and top gas amount and composition and surplus energy) for two stage smelting reduction process are presented here. The model is extended to blast furnace ironmaking to predict coke rate, top gas temperature, its composition and amount. These are also presented and compared with the data available from the plant.

4.1 TWO - STAGE SMELTING REDUCTION PROCESS

The calculations are made for a wide range of input variables in order to calculate coal rate, oxygen requirements, amount and composition of top, reduction gas and surplus reduction gas as a function of degree of metallization, post-combustion ratio, slag amount and coal grade. The results obtained from the model are given in Tables 4.1 - 4.14. The complete materials balances for the hot metal, slag, iron ore and coal can be seen in Tables 4.15 and 4.16. All these tables can be seen in Appendix X for quick reference. From thermal and chemical demand considerations, the following two cases are differentiated:

Case 1 : When only the MG thermal and chemical demand is met by coal combustion.

Case 2 : When thermal and chemical demand for both the reactors is met by coal combustion.

Thermal and chemical demands for various metallurgical operations typically at 0% and 100% metallization for 350, 450 and 550 kg/thm slag rates are given in Table 4.1.

Fig. 4.1a shows thermal and chemical demand for MG, RSF, case

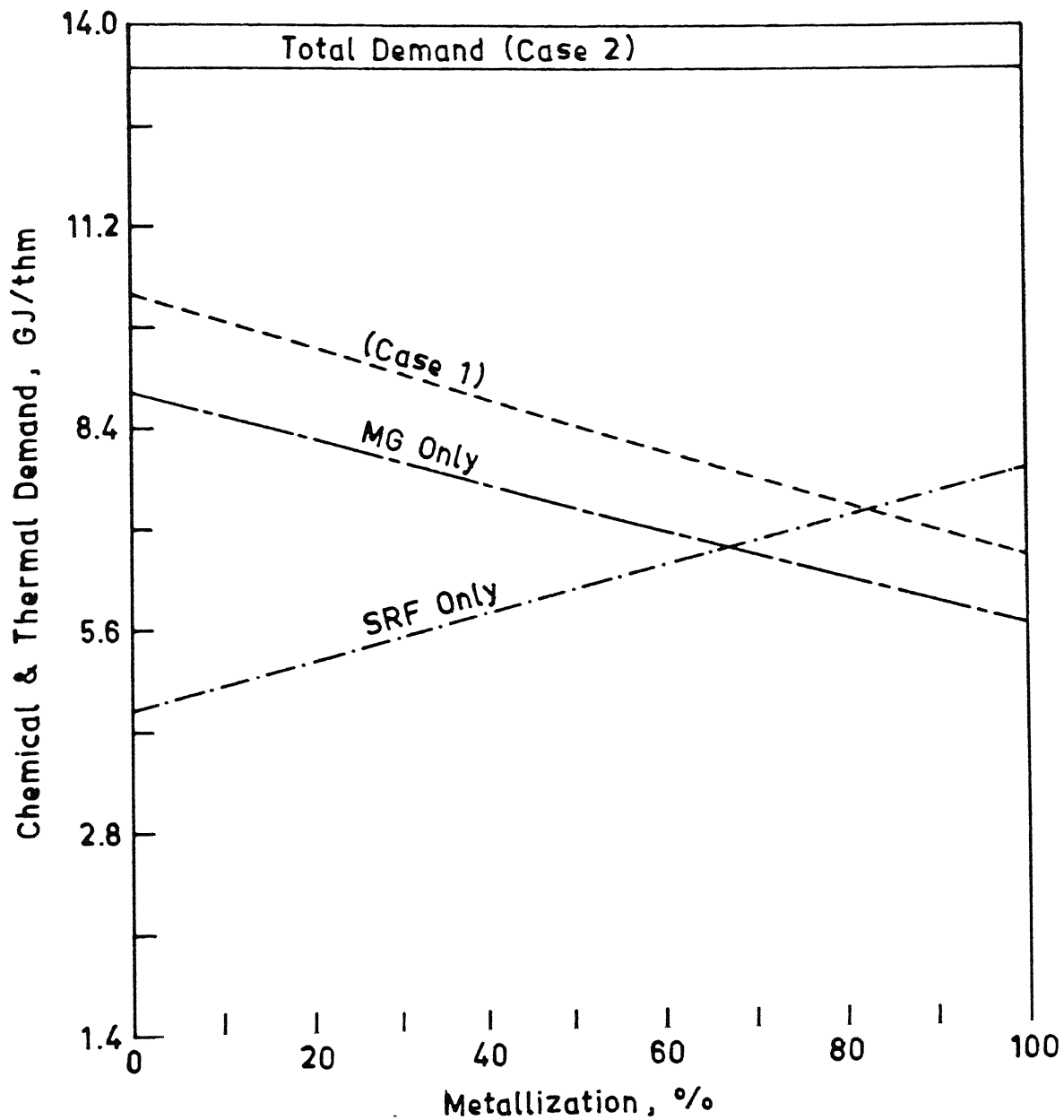


Fig. 4.1a Chemical and thermal demand vs the degree of metallization in RSF

1 and case 2 plotted against the degree of metallization in RSF for 450 kg/thm slag. As the degree of metallization in RSF increases from 0 to 100%, the thermal and chemical demand for RSF also increases from 4.49 to 7.77 GJ/thm because at higher degree of metallization more reduction of iron ore has to be carried out in the RSF. Thermal and chemical demand for the MG decreases from 8.95 to 5.67 GJ/thm as we increase the degree of metallization in RSF from 0 to 100% because less reduction of pre-reduced iron oxide is done now. At 100% metallization, the melter-gasifier carries out no reduction of iron oxide, so thermal and chemical demand for the MG is minimum here (5.67 GJ/thm). Thermal and chemical demand for case 1 includes sensible heat of the reduction gas also which decreases from 1.34 (10% of the overall thermal and chemical demand) to 1.07 (7.98 % of the overall thermal and chemical demand) as the degree of metallization in RSF increases from 0 to 100%. Since the amount of heat taken away from MG by the reduction gas decreases with the increase in metallization, the line for case 1 does not remain parallel to the line for MG thermal and chemical demand.

The total thermal and chemical demand for both the reactors (case 2) does not vary with the degree of metallization. Total thermal and chemical demand for both reactors remains constant (13.4 GJ/thm) because the sum of thermal and chemical demand for MG and RSF does not vary with the degree of metallization (eg. at 0% metallization, $8.95 + 4.49 = 13.44$ and at 100% metallization, $5.67 + 7.77 = 13.44$ GJ/thm). The values of energy for various metallurgical operations in the two-stage smelting reduction process given in Table 4.1 have been represented on Sanky diagram [9] in fig. 4.1b.

ALL VALUES IN GJ/thm

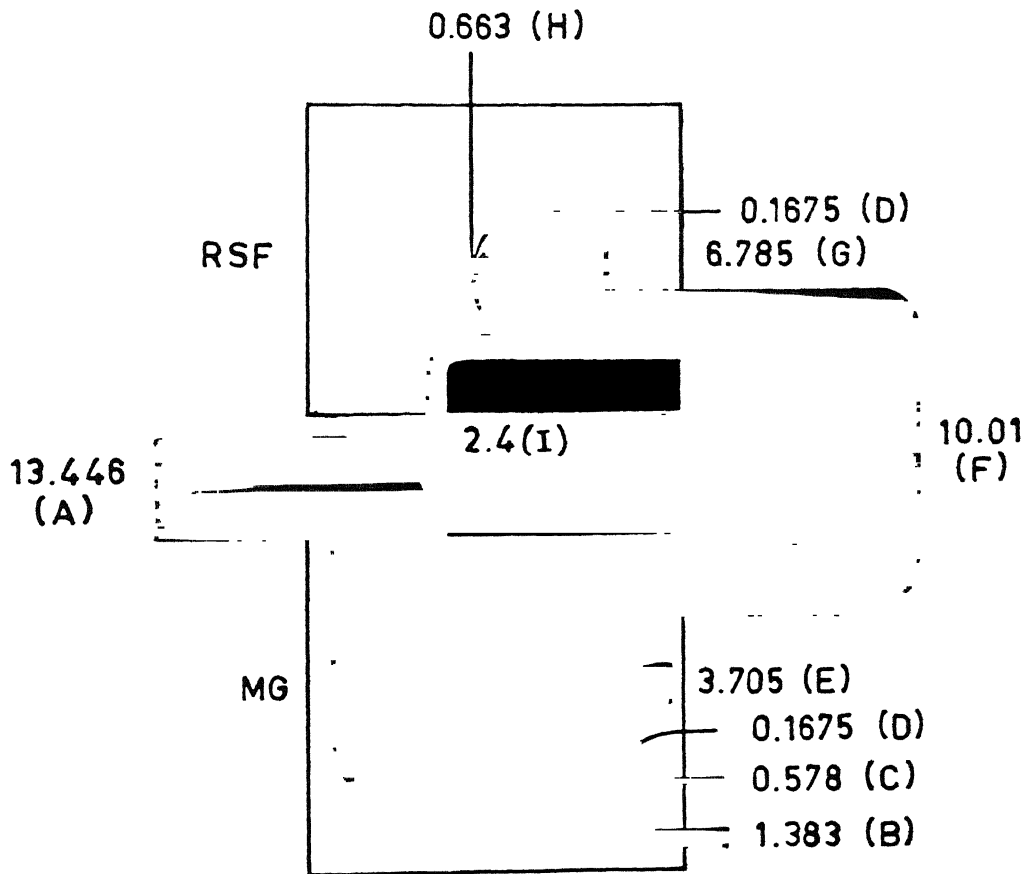


Fig. 4.1b Energy flow for two-stage smelting reduction process represented on Sanky diagram

A : COAL COMBUSTION
 B : HOT METAL
 C : SLAG
 D : LOSSES
 E : MG ENDOTHERMIC REACTIONS

F : REDUCTION GAS
 G : RSF ENDOTHERMIC REACTIONS
 H : TOP GAS
 I ; MATERIALS FROM RSF TO MG

4.1.1 Degree of Metallization

In the plots taken under this sub-head, the following are considered:

Slag rate = 450 kg/thm; ultimate analysis of bituminous coal (dry basis) : % C = 86.4, % H = 4.9, % O = 3.6, % N = 1.6, % S = 0.6 and % ash = 2.9; proximate analysis of coal: % VM = 22.2, % fixed C = 74.9 and % ash = 2.9)

The materials balance is presented in Table 4.15.

4.1.1.1 Coal Rate

In Fig. 4.2, coal consumption has been plotted against the degrees of metallization at various post combustion ratios for both cases. For case 1, coal consumption decreases from 1820.71 to 743.30 linearly (see Table 4.2) at 0% post-combustion as degree of metallization is increased from 0 to 100%. Similar trend is seen for other post-combustion ratios. This is due to the decreasing heat demand for case 1 with increasing degree of metallization (see Fig. 4.1, already discussed). Since heat demand for case 2 does not vary with the degree of metallization, coal consumption also remains constant. For 0% post-combustion this constant value of coal is 1852.23 (see Table 4.13). Similar trend has been seen for other post-combustion ratios for case 2.

At 0% metallization for 0% post-combustion, the difference between the coal consumption for both cases ($1852.23 - 1820.71 = 31.52$ kg/thm) is very small as compared to the difference at 100% metallization ($1852.23 - 743.30 = 1108.93$ kg/thm). Same trend is seen for other post combustion ratios. This is due to the fact that the heat demand for case 2 does not vary with the degree of metallization in RSF whereas case 1 heat demand decreases with the increase in the degree of metallization in RSF. The cumulative

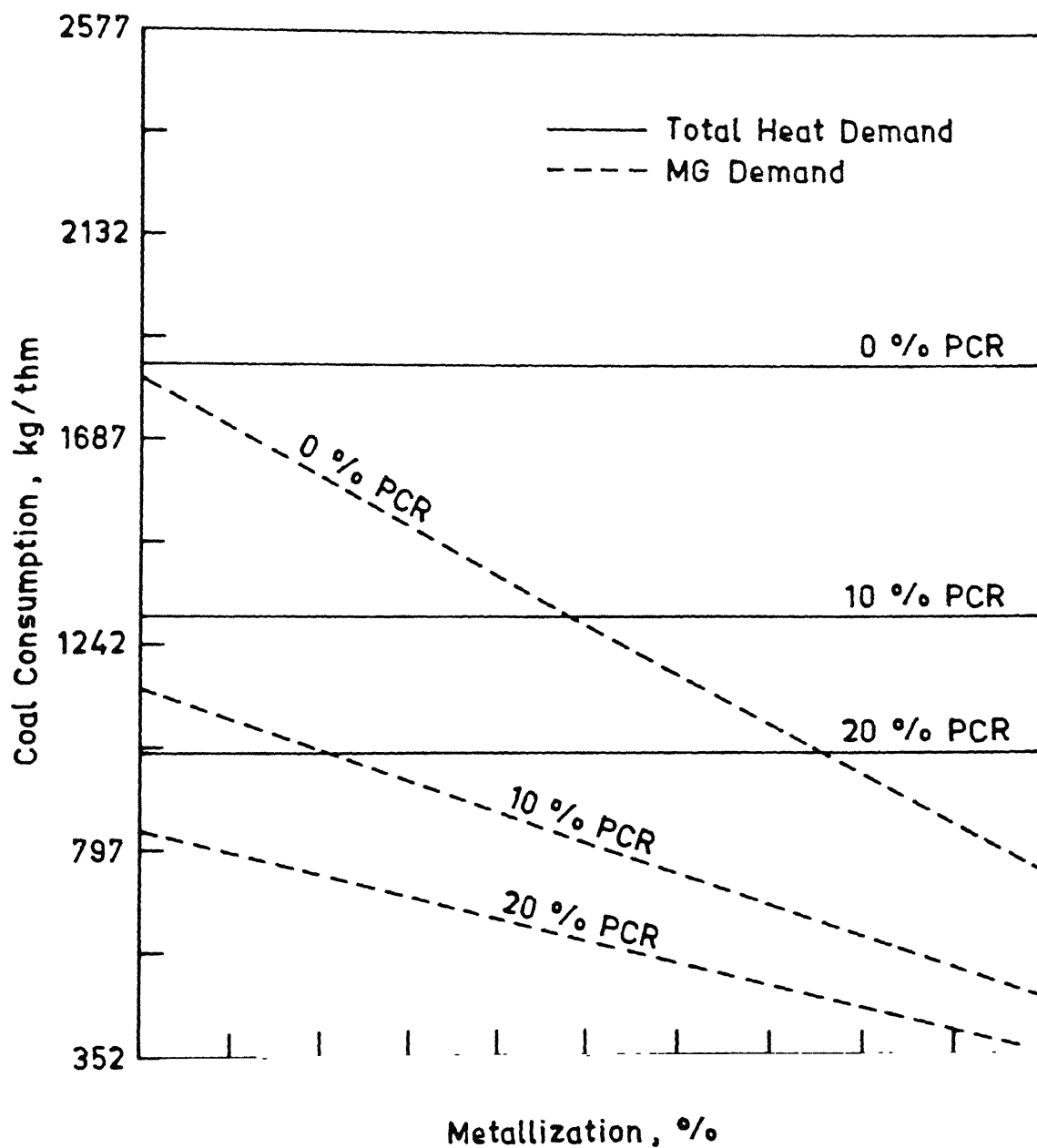


Fig. 4.2 Coal consumption vs. the degree of metallization at various post-combustion ratios for both cases

effect is to increase the difference between the coal consumption for two cases.

4.1.1.2 O_2 Requirement and $(CO + H_2)$ production

Since oxygen requirement and production of reduction gas is directly proportional to coal consumption and because coal consumption decreases with the increase in degree of metallization in RSF, oxygen requirement and production of reduction gas will also decrease with the increase in the degree of metallization in RSF for case 1. This observation for oxygen is shown in Fig. 4.3 and Table 4.4. At 0% post-combustion, for 0% metallization the O_2 requirement for coal combustion is $2524.95 \text{ Nm}^3/\text{thm}$ and for 100% metallization it is $1013.24 \text{ Nm}^3/\text{thm}$. The variation is linear. Similarly, $(CO + H_2)$ production decreases linearly from 3929.21 to $1600.29 \text{ Nm}^3/\text{thm}$ for 0% when the degree of metallization in RSF increases from 0 to 100% for case 1 (see Fig. 4.4 and Table 4.6). For case 2, O_2 requirement for coal combustion and $(CO + H_2)$ production remains constant for all degrees of metallization at a particular post - combustion ratio. For case 2, at 0% post-combustion O_2 requirement for coal combustion is $2575 \text{ Nm}^3/\text{thm}$ (see Fig. 4.3 and Table 4.13) whereas $(CO + H_2)$ production is $3997.35 \text{ Nm}^3/\text{thm}$ (see Fig. 4.5 and Table 4.13). The trend for other post combustion ratios remains to be the same. The reduction gas with post-combustion consists of CO , CO_2 , H_2 , H_2O and N_2 and without post-combustion, it consists of CO , H_2 and N_2 . In Fig. 4.4 and 4.5, only reducing gases i.e. CO and H_2 amounts have been taken after subtracting the amount of non-reducing gases (i.e. CO_2 , H_2O and N_2) from the total reduction gas amount.

4.1.1.3 Surplus Gas

The variation of surplus reduction gas with the degree of

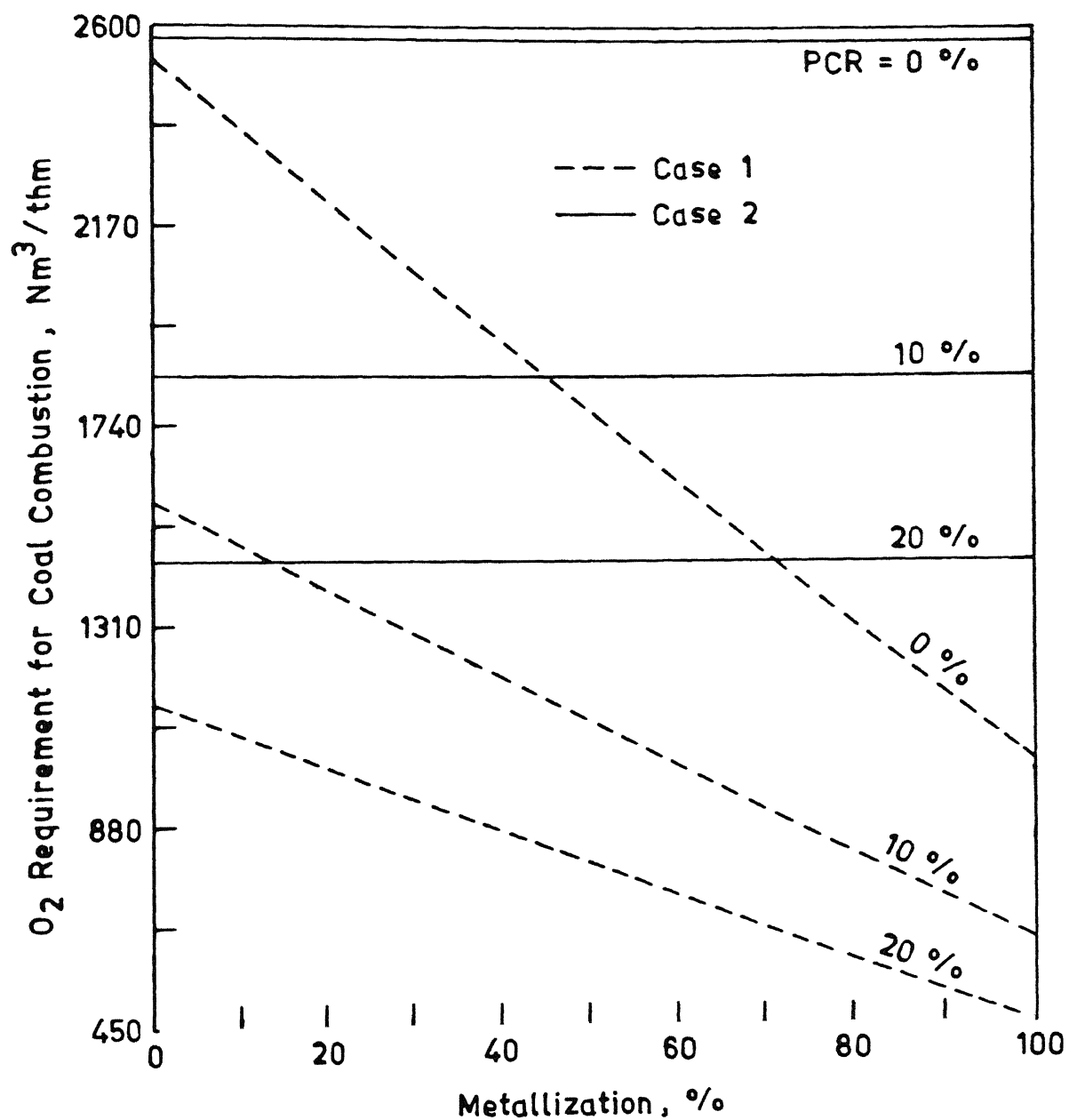


Fig. 4.3 O_2 requirement for coal combustion vs the degree of metallization at various post combustion ratios for both cases

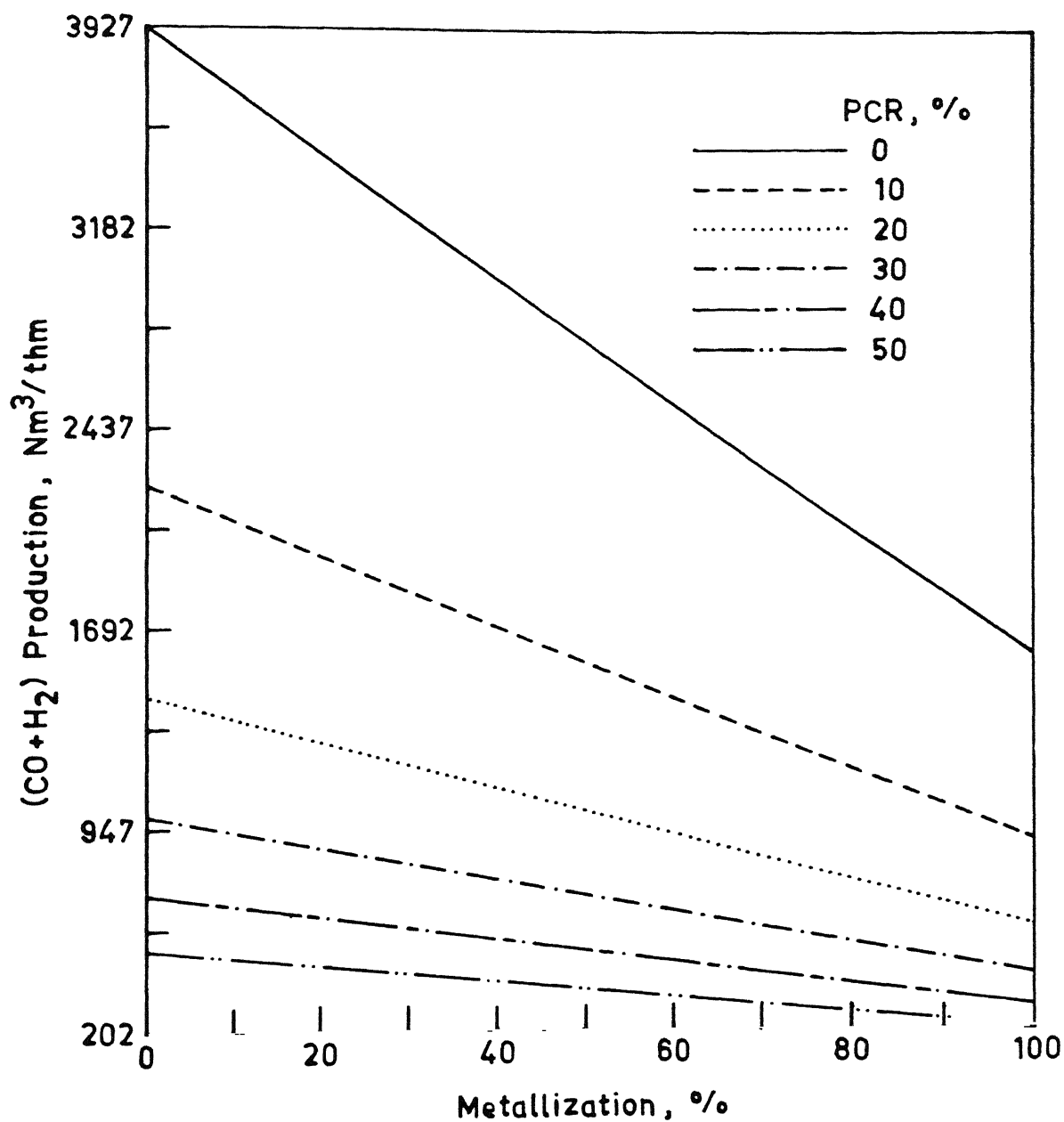


Fig. 4.4 (CO + H₂) production vs. the degree of metallization at various post combustion ratios for case 1

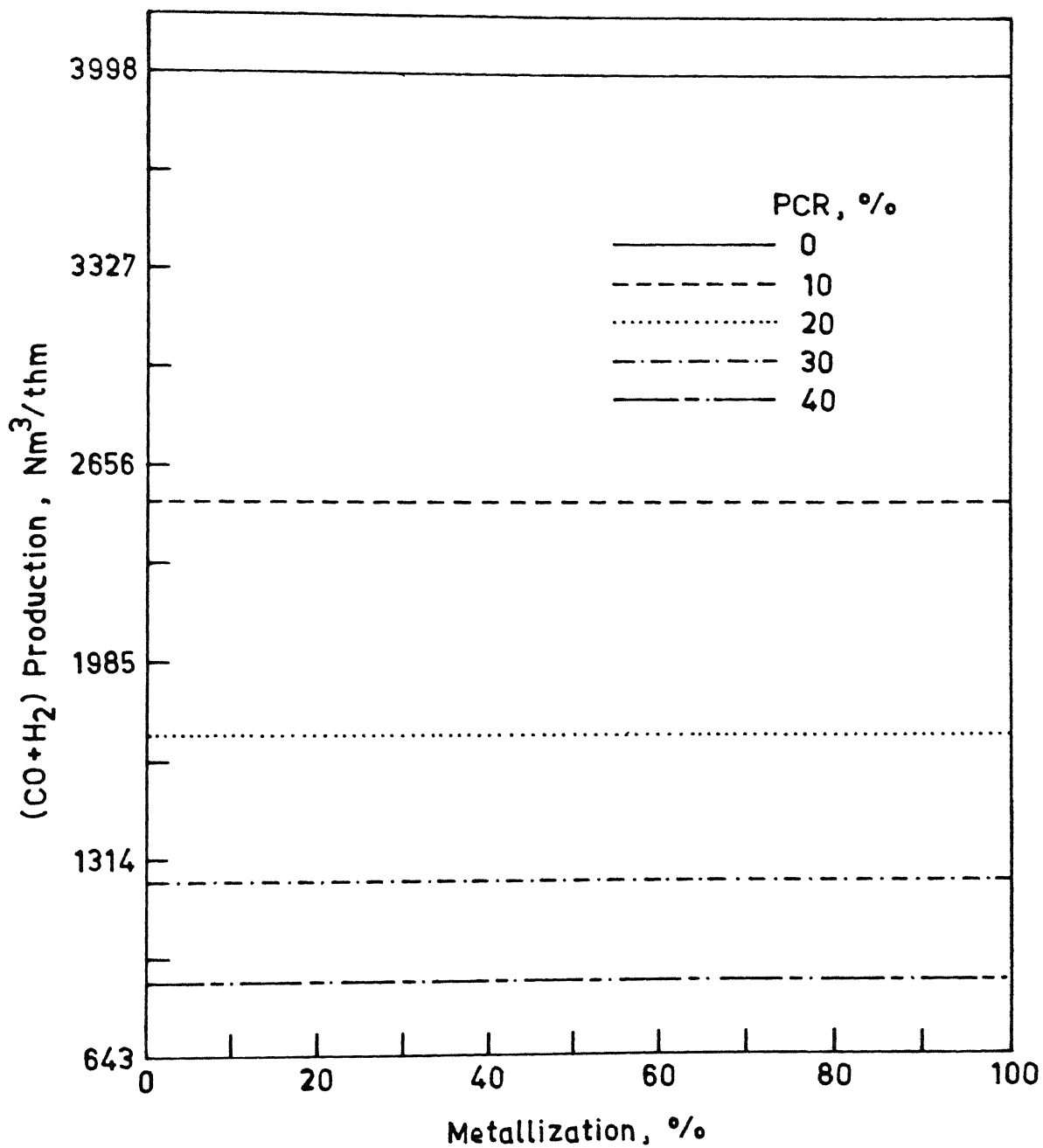


Fig. 4.5 (CO + H₂) production vs the degree of metallization at various post-combustion ratios for case 2

metallization in the RSF is plotted in Fig. 4.6 and 4.7 for case 1 and case 2 for various post-combustion ratios.

$$\left(\begin{array}{c} \text{Surplus} \\ \text{reduction} \\ \text{gas} \end{array} \right) = \left(\begin{array}{c} \text{Production} \\ \text{of } (\text{CO} + \text{H}_2) \\ \text{in the MG} \end{array} \right) - \left(\begin{array}{c} \text{Chemical requirement} \\ \text{of } (\text{CO} + \text{H}_2) \text{ in} \\ \text{RSF} \end{array} \right)$$

In Fig. 4.8, $(\text{CO} + \text{H}_2)$ requirement for pre-reduction in RSF and $(\text{CO} + \text{H}_2)$ production in the MG are plotted together against the degree of metallization for various post-combustion ratios. The figure is valid for case 1 only. The $(\text{CO} + \text{H}_2)$ requirement has been calculated from $\text{Fe}_{0.95}\text{O} - \text{Fe}$ thermodynamic equilibrium at 1200 K. $(\text{CO} + \text{H}_2)$ left after $\text{Fe}_{0.95}\text{O} - \text{Fe}$ reaction is sufficient enough to carry out $\text{Fe}_2\text{O}_3 - \text{Fe}_3\text{O}_4$ and $\text{Fe}_3\text{O}_4 - \text{Fe}_{0.95}\text{O}$ reactions upto a certain degree of metallization (known as critical metallization). It is 33.46% for 0% PCR line as shown in fig. 4.8 by the arrow mark. $(\text{CO} + \text{H}_2)$ requirement increases with the increasing post-combustion as less H_2 will be available for the replacement of CO.

As is clear from Fig. 4.8 that an increase in the degree of metallization results in the decrease in production of $(\text{CO} + \text{H}_2)$ (explained earlier) and increase in $(\text{CO} + \text{H}_2)$ requirement. The cumulative effect is that the surplus reduction gas (i.e. production of $\text{CO} + \text{H}_2$ - requirement of $\text{CO} + \text{H}_2$) decreases from 3520.52 to 379.08 Nm^3/thm as degree of metallization in RSF increases from 0 to 100%. (See Table 4.8 for corresponding calorific values of the surplus reduction gas). Similar trend is observed for case 2 for all post combustion ratios.

Calorific value of the gas has been calculated by considering complete combustion of CO and H_2 to CO_2 and H_2O respectively.

4.1.1.4 Top Gas

Since 30% utilization of CO and 37% utilization of H_2 is

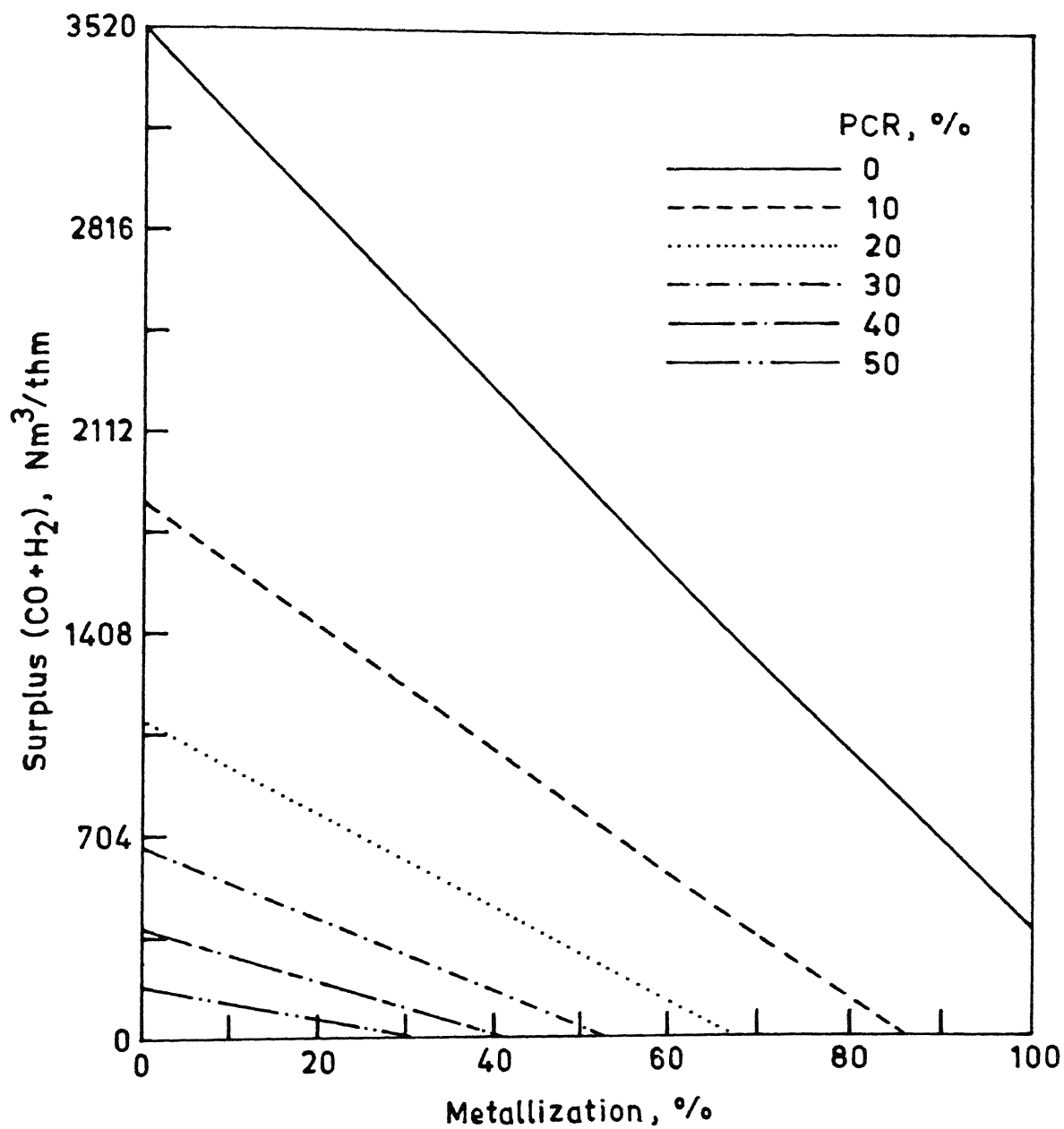


Fig. 4.6 Surplus reduction gas vs. the degree of metallization at various post combustion ratios for case 1

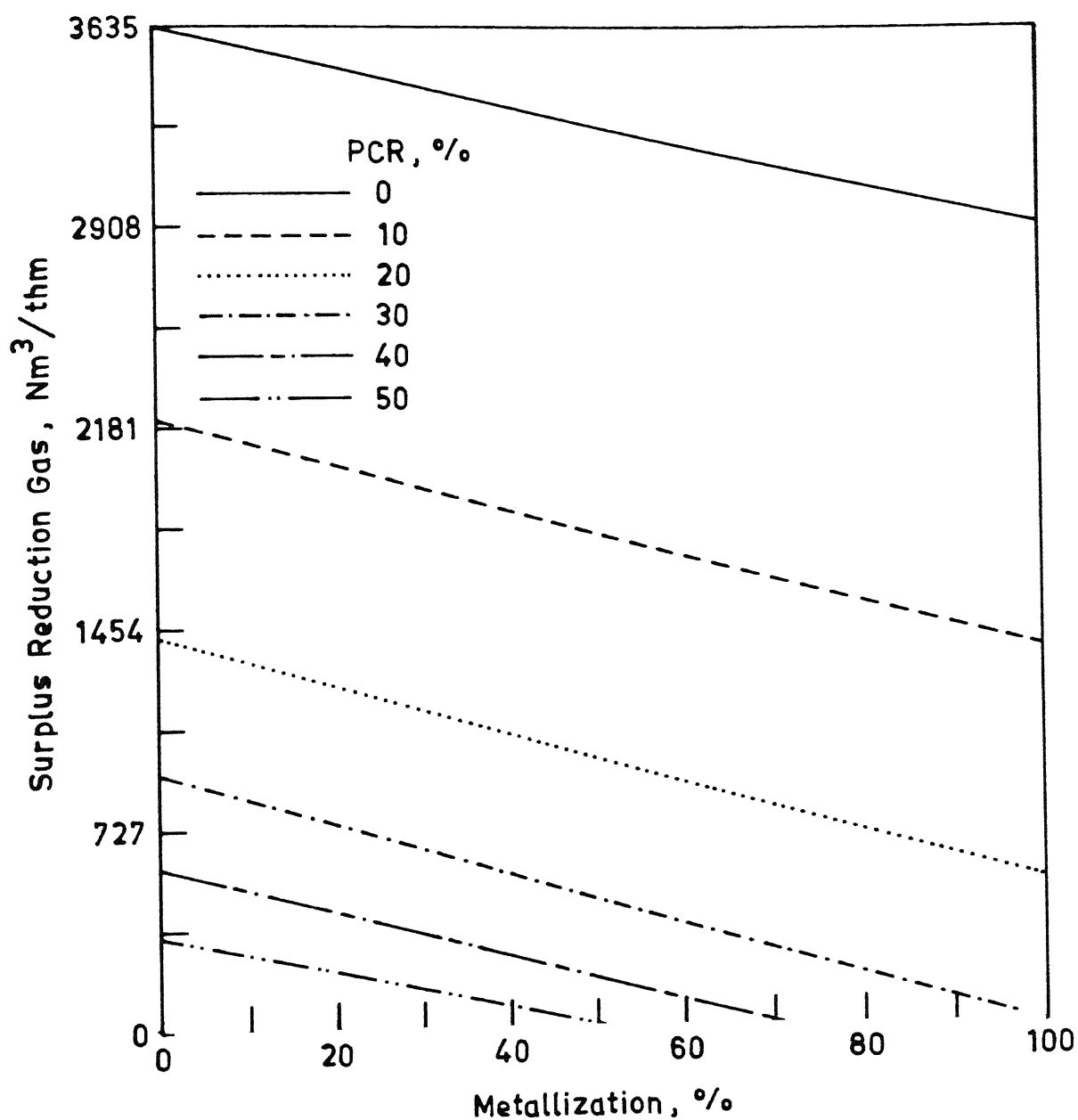


Fig. 4.7 Surplus reduction gas vs. the degree of metallization at various post combustion ratios for case 2

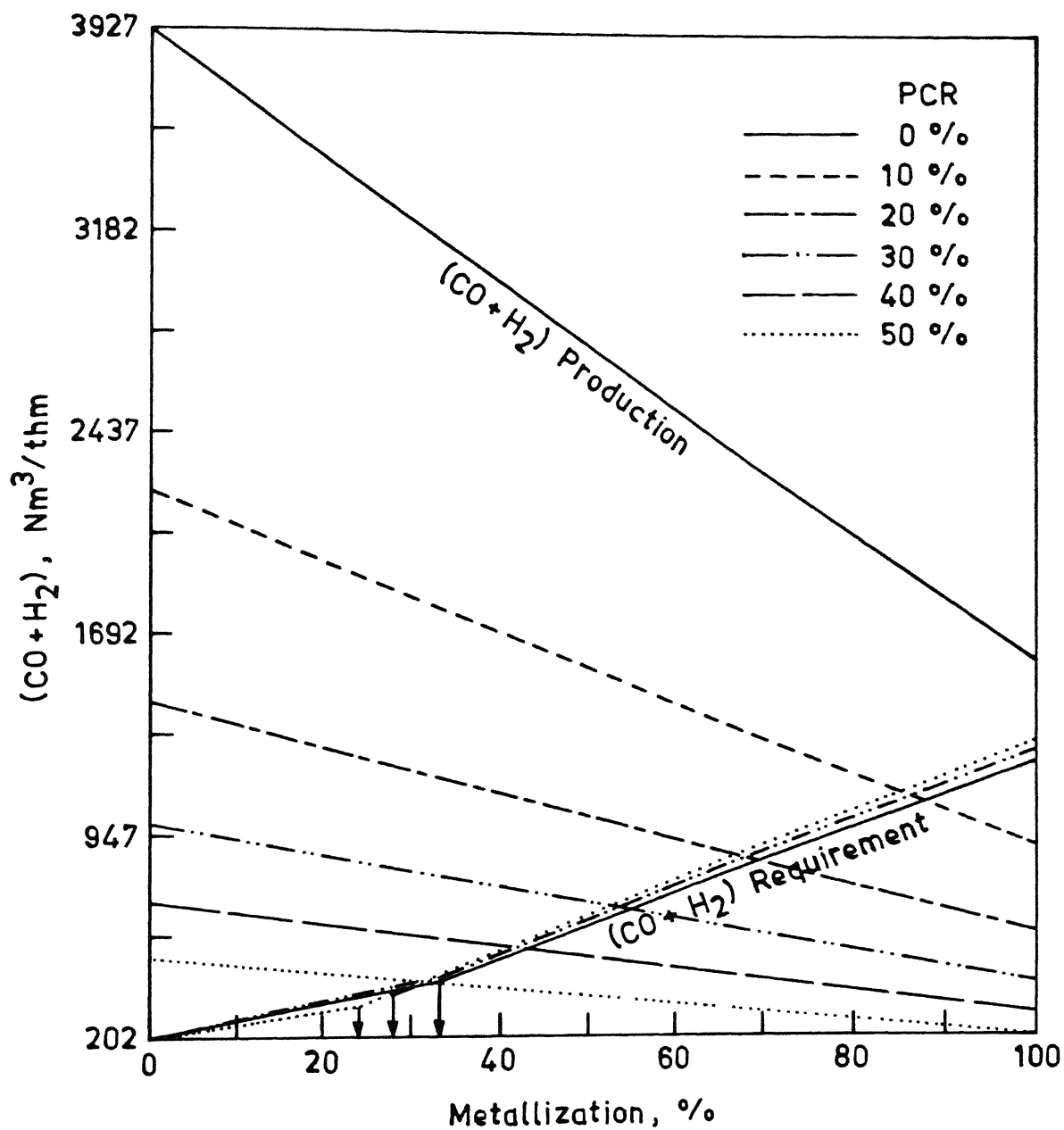


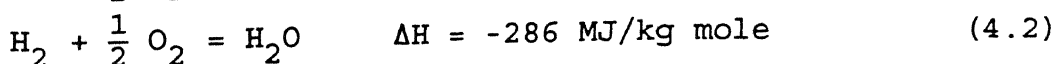
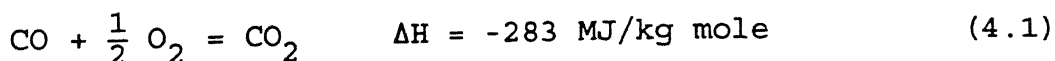
Fig. 4.8 $(CO + H_2)$ requirement and production vs degree of metallization at various post combustion ratios for case 1

considered at 1200 K for $\text{Fe}_{0.95}\text{O}$ -Fe equilibrium, the top gas will consist of large amounts of CO and H_2 . As degree of metallization increases, $(\text{CO} + \text{H}_2)$ requirement increases. So, an increase in amount and hence its calorific value of the top gas is expected as degree of metallization increases. Reduction gas should have sufficient reduction potential to pre-reduce iron ore therefore it is scrubbed (i.e. CO_2 and H_2O portion of the gas is removed from it) before it enters the RSF. Since only the amount of $(\text{CO} + \text{H}_2)$ required for pre-reduction is sent to the RSF, there is no differentiation between case 1 and case 2. For 0% post-combustion, $(\text{CO} + \text{H}_2)$ amount increases from $278.116 \text{ Nm}^3/\text{thm}$ (12.9 GJ/thm) to 832.73 (23.6 GJ/thm) as we move from 0% to 100% metallization in RSF (see Table 4.10). Same trend is seen for other post combustion ratios. Top gas composition when the reduction gas after scrubbing is sent to the RSF is presented in Table 4.11.

4.1.2 Post Combustion

For the plots taken under this sub-head slag rate is 450 kg/thm and bituminous coal (same as in previous case) has been used.

The gases produced during the combustion of coal in the MG are at or nearly thermal and chemical equilibrium with the hot metal which is around 1700 - 1850 K with a relatively high C content (3-4%) therefore stable form of oxide of C is monoxide and hydrogen will exist as element. The post-combustion of H_2 and CO in the melter - gasifier is a very useful method of reducing coal consumption, since the combustion reaction (Equations 4.1 and 4.2)



are highly exothermic in nature. For the post-combustion of the reducing gas, the necessary O_2 is injected from the top of the melter-gasifier which needs a suitable technological arrangement. Need for good refractory lining also gets enhanced due to higher flame temperature generated in the top of the melter gasifier. Flame temperatures for different degrees of post combustion have been given in Table 4.17. CO_2 and H_2 generated by combustion of CO absorbs all the heat generated and appears as a flame. Because of high amount of heat absorbed its temperature increases which is known as flame temperature. This can be calculated as follows:

From reaction (4.1) and (4.2), we have



$$\begin{aligned} & (\text{Kg mole of } CO_2) \cdot (C_p \text{ of } CO_2) (T_{\text{flame}} - 1273) + \\ & (\text{kg mole of } H_2O) (C_p \text{ of } H_2O) (T_{\text{flame}} - 1273) = 286000 (\text{kg} \\ & \text{mole of } H_2 \text{ in the reduction gas}) + 283000 (\text{kg mole of CO in} \\ & \text{the reduction gas}) \end{aligned} \quad (4.3)$$

Table 4.17 : Flame temperatures for various post-combustion ratios

PCR (%)	Flame Temperature (K)
0	1273.00
10	1768.72
20	2264.44
30	2760.17
40	3255.89
50	3751.62

To take care of the refractory lining, tuyere flame temperature can be lowered by using air instead of pure O_2 for post-combustion.

4.1.2.1 Coal Rate

The additional heat generated due to post-combustion should result in the reduction in the coal consumption which is confirmed by Fig. 4.9.

In Fig. 4.9, the coal consumption is plotted against post combustion ratio at 0, 30, 60 and 90% metallization for case 1. Since coal rate for case 2 does not depend on the degree of metallization, we get only one line for all degrees of metallization.

The coal consumption decreases with the post - combustion ratio for both cases. Consider the operation of the process for 0% metallization 0% metallization corresponds to reduction of Fe_2O_3 to wustite only in the reduction shaft furnace. Since no iron forms in the reduction shaft furnace, no sticking [17] of iron particles occur in the reduction shaft furnace and during conveying of the pre-reduced burden into the melter gasifier via screw-conveyor. So, technological advantage of using fine ore in the charge can be obtained at 0% metallization. In this case, the melter-gasifier operates under highly reducing conditions the intensity of which depends on the post-combustion ratio. Intensity of reducing conditions decreases as well increase the post combustion ratio because coal combustion decreases.

For 90% metallization, the coal consumption is minimum (851.04 kg/thm at 0% PCR and 271.21 kg/thm at 50% PCR) as compared to the other degrees of metallization (see Table 4.2). Here sufficient Fe forms in the reduction shaft furnace which leads to sticking. In order to avoid sticking, technologies such as fluidized bed reduction have been employed. Operations for 30% and 60% metallization fall between the two extreme operations for

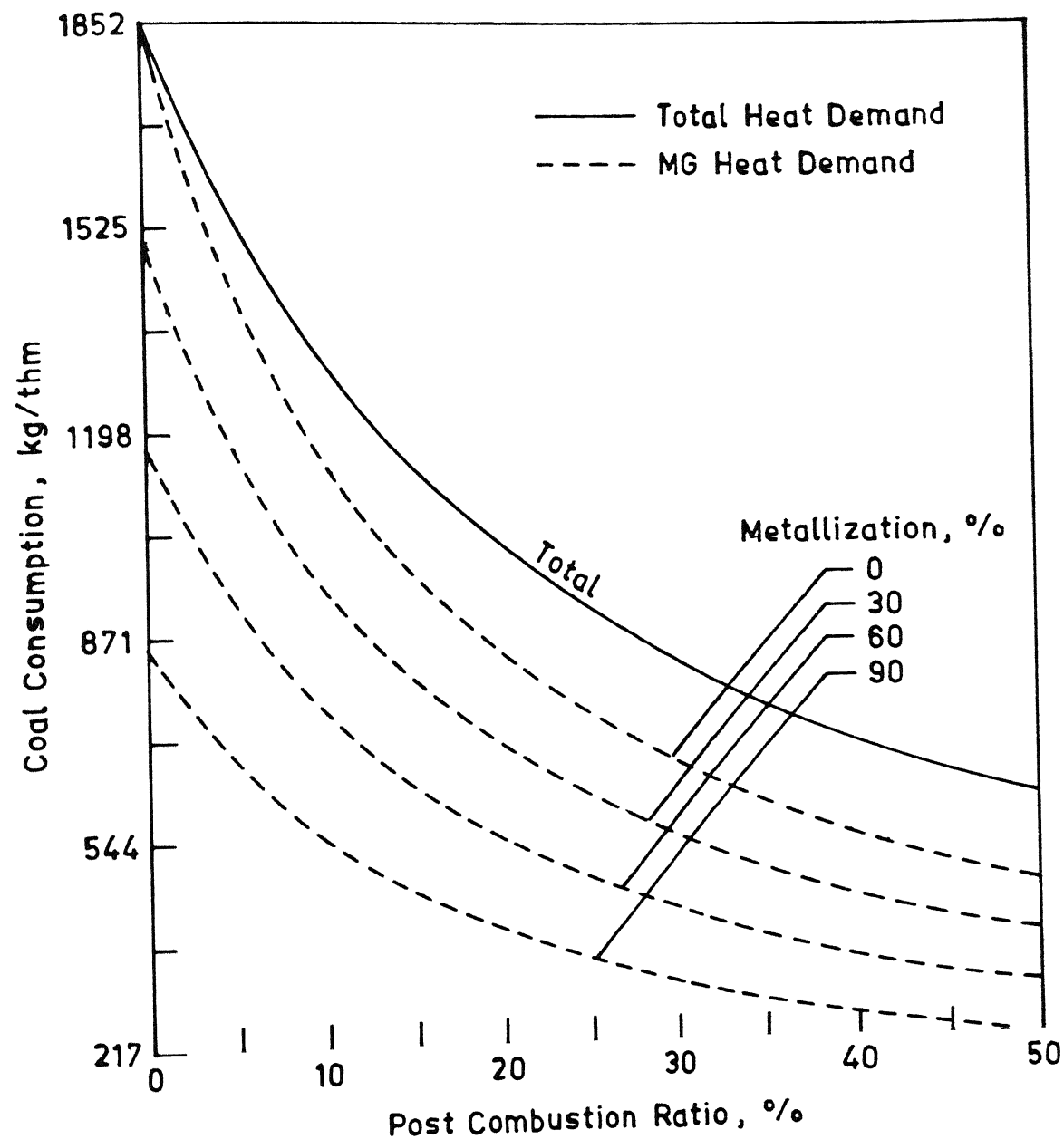


Fig. 4.9 Coal consumption vs. post combustion ratio at various degrees of metallization for both cases

0% and 100% metallization.

Consider the operation of the process for 90% metallization with varying post-combustion ratio. This operation at 0% PCR is similar to the existing COREX process.

For 0% PCR the coal consumption at 90% metallization is 851.04 kg/thm whereas it is 462.19 kg/thm for 50% PCR and 0% metallization (for case 1). This means for 0% PCR at 90% metallization, we will have strong reducing conditions. This will increase the reduction of SiO_2 to Si as a consequence of which Si content of the hot metal will increase. So, for a fixed Si content of the hot metal, ash content of coal and gangue content of ore should be suitably selected in the COREX process.

4.1.2.2 ($\text{CO} + \text{H}_2$) production and O_2 requirement

If the post-combustion is very high, the reduction gas will not have enough reduction potential to obtain the degree of metallization desired. For example for 30% PCR (see Table 4.12), CO utilization = $22.2 / (51.83 + 22.2) = 30\%$ so reduction gas has no sufficient reduction potential for $\text{Fe}_{0.95}\text{O} - \text{Fe}$ equilibrium at 1200 K above this post-combustion ratio.

However it is possible to remove CO_2 and H_2O from the reduction gas by gas scrubbing. CO and H_2 left after the scrubbing operation have sufficient reduction potential to carry out the desired degree of metallization in the reduction shaft furnace. However additional energy would be required ($\sim 4800 \text{ KJ/Nm}^3 \text{ CO}_2$) for scrubbing operation [22]. For calculations, the component of the reduction gas left after scrubbing (i.e. $\text{CO} + \text{H}_2$) is considered to be sent to the reduction shaft furnace.

O_2 required for coal combustion and O_2 required for post-combustion have been plotted against post-combustion ratio

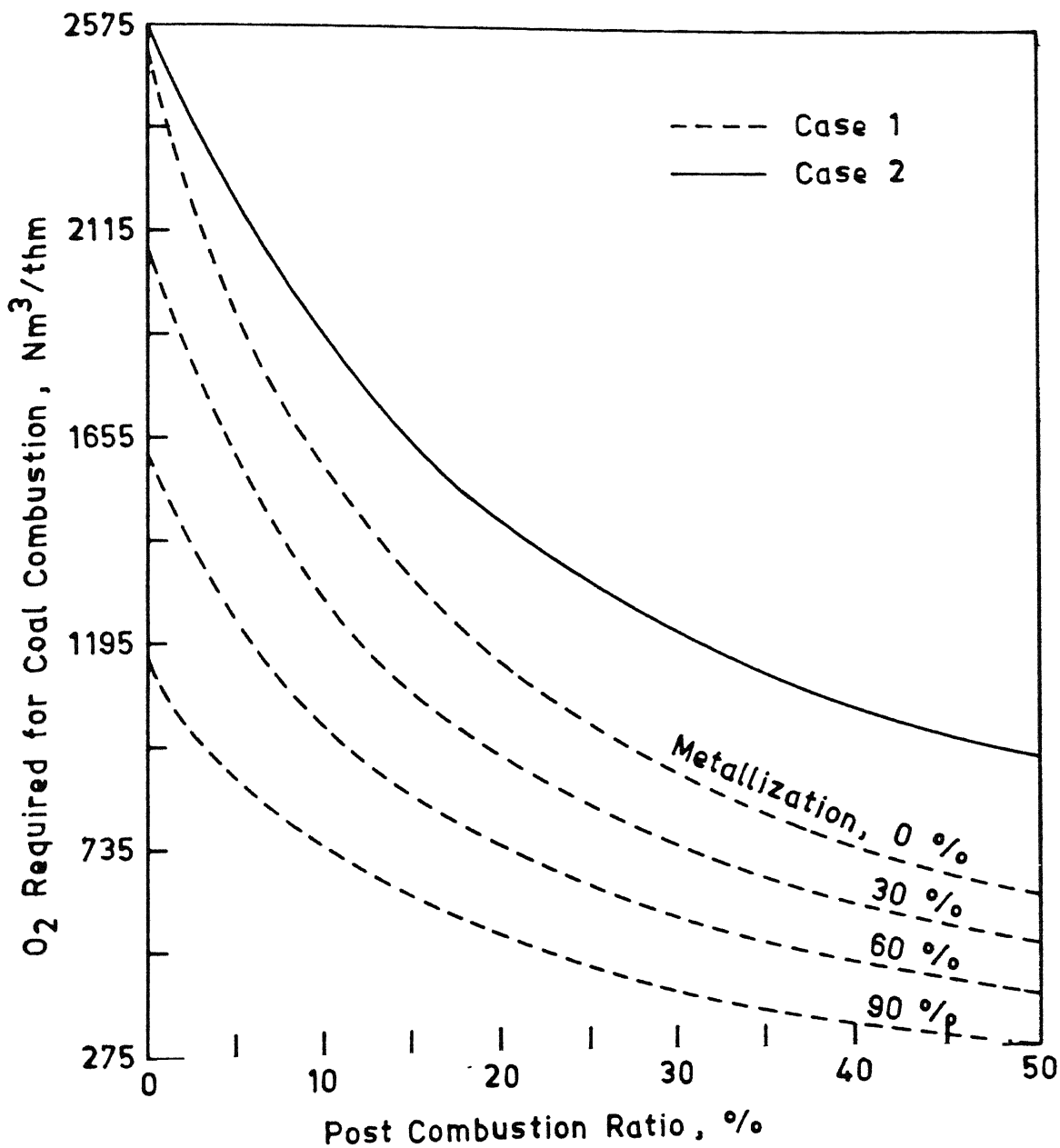


Fig. 4.10 O_2 requirement for coal combustion vs post-combustion ratio at various degrees of metallization for both cases

for various degrees of metallization in Fig. 4.10 and 4.11 respectively. O_2 requirement for coal combustion decreases with the increase in post-combustion ratio whereas O_2 requirement for post combustion increases with the increase in PCR for all degrees of metallization.

Decrease in O_2 requirement for coal combustion is much faster than the increase in O_2 requirement for post-combustion. This can be seen from Table 4.4. For a difference of 10% in post-combustion ratio at 0% metallization for case 1, the O_2 requirement for coal combustion falls from 2524.95 to 1575.66 Nm^3/thm (difference = 949.29 Nm^3/thm) whereas O_2 requirement for post-combustion rises from 0 to 123.43 Nm^3/thm (difference = 123.43 Nm^3/thm). The result being that the total O_2 requirement decreases with post-combustion ratio. Same trend is observed for other % metallization in RSF and case 2. Since case 2 does not depend on the degree of metallization in RSF, we get only one line for all degrees of metallization.

4.1.2.3 Surplus Gas

As the degree of post-combustion increases, $(CO + H_2)$ production decreases (because coal consumption decreases) which was obvious from Fig. 4.4 and 4.5 whereas requirement does not change much (see Fig. 4.8). So, decrease in surplus reduction gas $(CO + H_2)$ amount and hence its calorific value is expected with the increase in post-combustion ratio for various degrees of metallization for both cases. This has been confirmed by Fig. 4.12 for case 1 and case 2 (also see Table 4.8).

For case 1, at 0% metallization in RSF and at 0% post-combustion the surplus reduction gas calorific value is 49.7 GJ/thm, as amount of post-combustion increases to 10% and 20% this

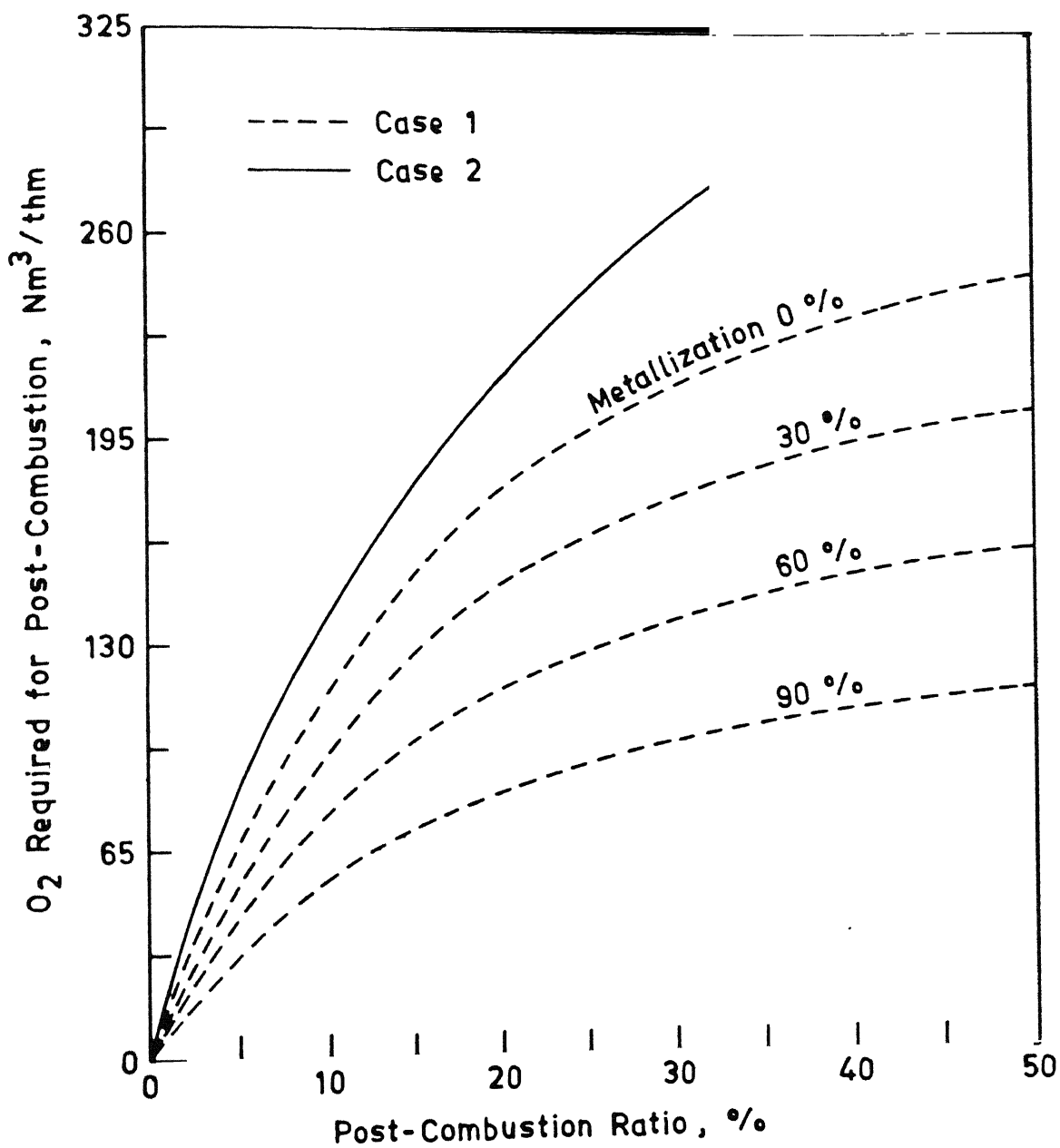


Fig. 4.11 O_2 requirement for post combustion vs post-combustion ratio at various degrees of metallization for both cases

value decreases to 28.1 GJ/thm and 18.2 GJ/thm respectively. This decrease in the calorific value with increase in post-combustion ratio is seen for other degrees of metallization and case 2 also. The reason for this decrease in calorific value of the surplus reduction gas is that after the post-combustion, we get less amount of reducing gases ($\text{CO} + \text{H}_2$) because a portion of reducing gases ($\text{CO} + \text{H}_2$) gets post-combusted to CO_2 and H_2O respectively. Now in Fig. 4.12, see the line for case 1 at 90% metallization - we get 16.5 GJ/thm surplus reduction gas at 0% post combustion and 0GJ/thm at 27.5% post - combustion ratio. This means that at 90% metallization for 27.5% post-combustion, no surplus reduction gas is available (i.e. production of $\text{CO} + \text{H}_2$ = Chemical requirement of $\text{CO} + \text{H}_2$).

When in a plant, it is not required to use the surplus reduction gas to run separate facilities available in the plant like DRI production unit, pelletizing plant, power plant etc., the two stage smelting reduction process is operated at an optimum metallization. At optimum metallization, the production of ($\text{CO} + \text{H}_2$) in the melter gasifier is equal to the chemical requirement of ($\text{CO} + \text{H}_2$) in the reduction shaft furnace i.e the operation is matched one. Since no surplus reduction gas is available at this point, the coal consumption will be minimum at this point.

In Fig. 4.8, at the point of intersection of the lines for production of ($\text{CO} + \text{H}_2$) and its requirement, we don't get any surplus reduction gas. This point of intersection of the two lines is the optimum metallization. If the process is operated at a point below the optimum metallization, some surplus reduction gas can be taken out of the process as production of ($\text{CO} + \text{H}_2$) is greater than chemical requirement. Since at 0% PCR, the amount of

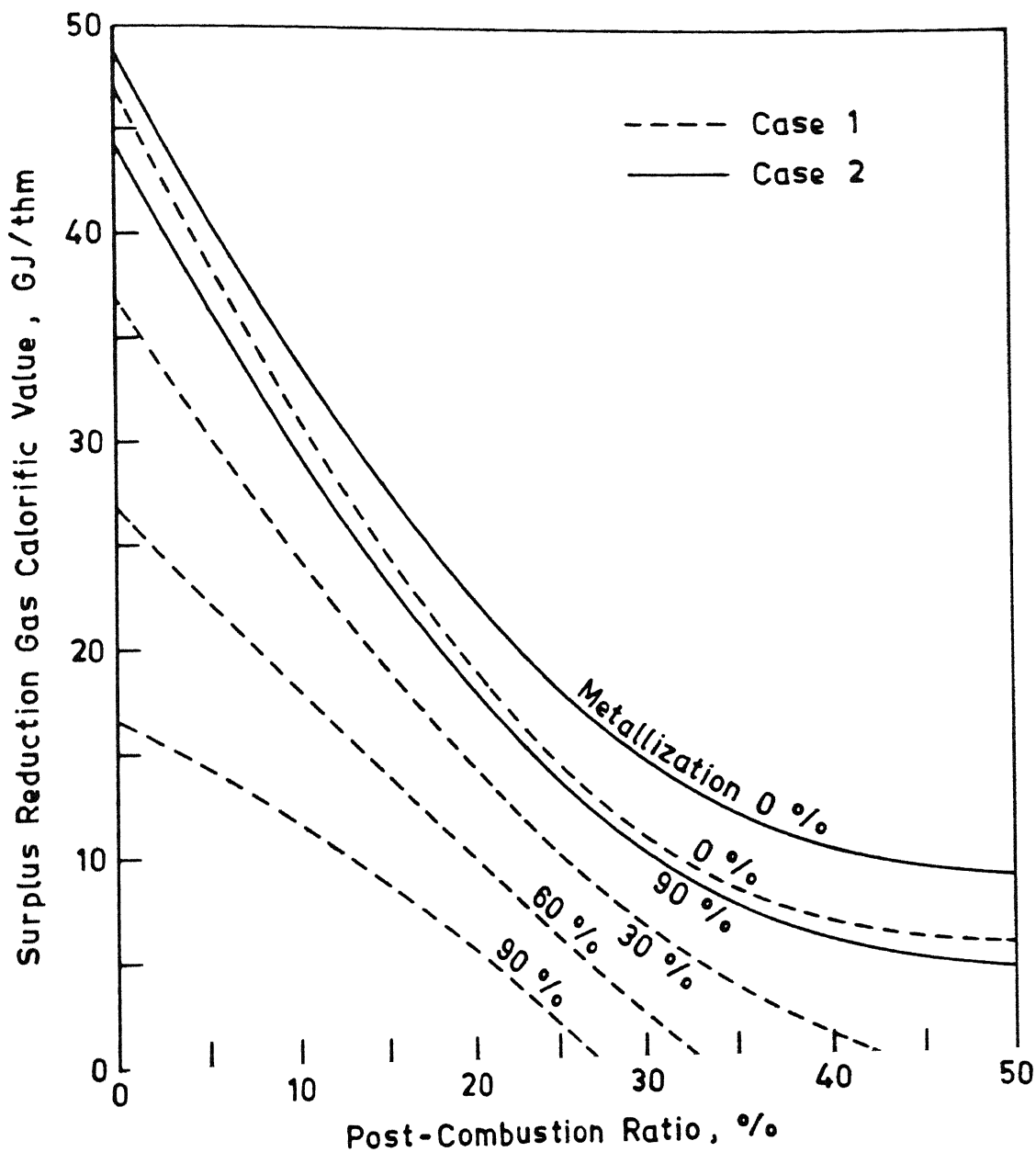


Fig. 4.12 Surplus reduction gas calorific value vs post-combustion ratio at various degrees of metallization for both cases

$\text{CO} + \text{H}_2$ in the reduction gas leaving the melter gasifier is very high, the point at which production and requirement lines meet (i.e the optimum point) also becomes very high. Lines for 0% PCR meet at 110.67 if extended beyond 100% metallization (since it is impossible to carry out such a degree of metallization, it is called an imaginary optimum point). Significance of the points above 100% metallization is that surplus reduction gas will be available for all degrees of metallization in RSF.

To decrease the optimum degree of metallization post-combustion of the reducing gas ($\text{CO} + \text{H}_2$) is necessary in the MG. As the degree of post-combustion increases, the ($\text{CO} + \text{H}_2$) produced in the MG decreases. So, the lines for production shift towards bottom left, which results in decrease in optimum metallization with the degree of post-combustion. This information can be derived from Fig. 4.8. For 10, 20, 30% post-combustion ratios the optimum metallization in RSF drops down to 86.14, 67.45 and 52.74% respectively.

4.1.3 Slag Amount

An increase in slag amount can occur due to increase in gangue content of the ore, ash content of the coal and CaCO_3 consumption. Calculations are performed for fixed hot metal amount and composition, fixed slag composition, constant basicity of the slag, fixed % ash in coal, fixed ash composition and for pure CaCO_3 .

In the plots taken under this sub-head, post-combustion ratio = 0% and bituminous coal of following composition has been taken :

(Dry basis)

%C = 86.4,	%H = 4.9,	%O = 3.6
% N = 1.6,	%S = 0.6	& % ash = 2.9

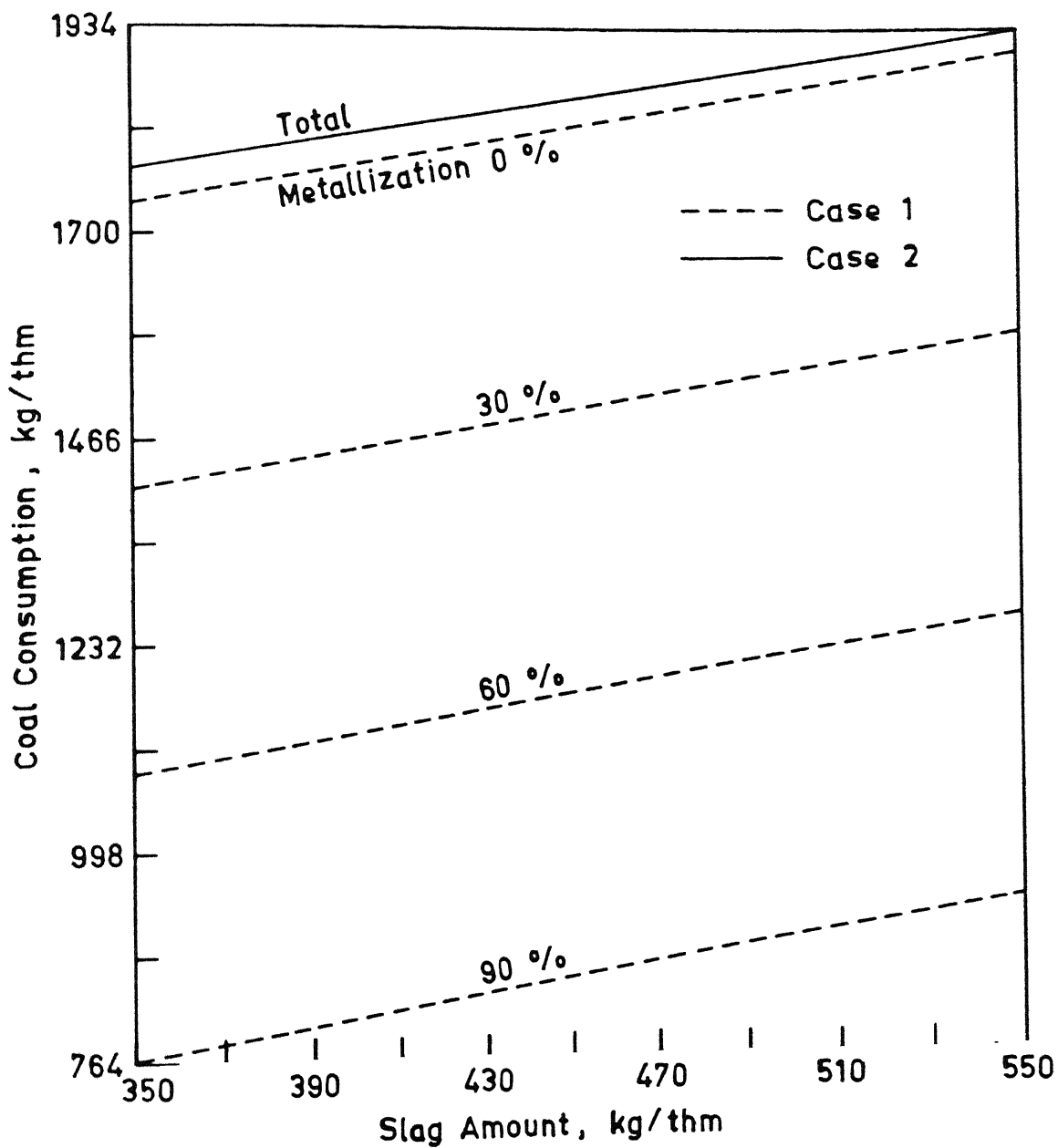


Fig. 4.13 Coal consumption vs slag amount at various degrees of metallization for both cases

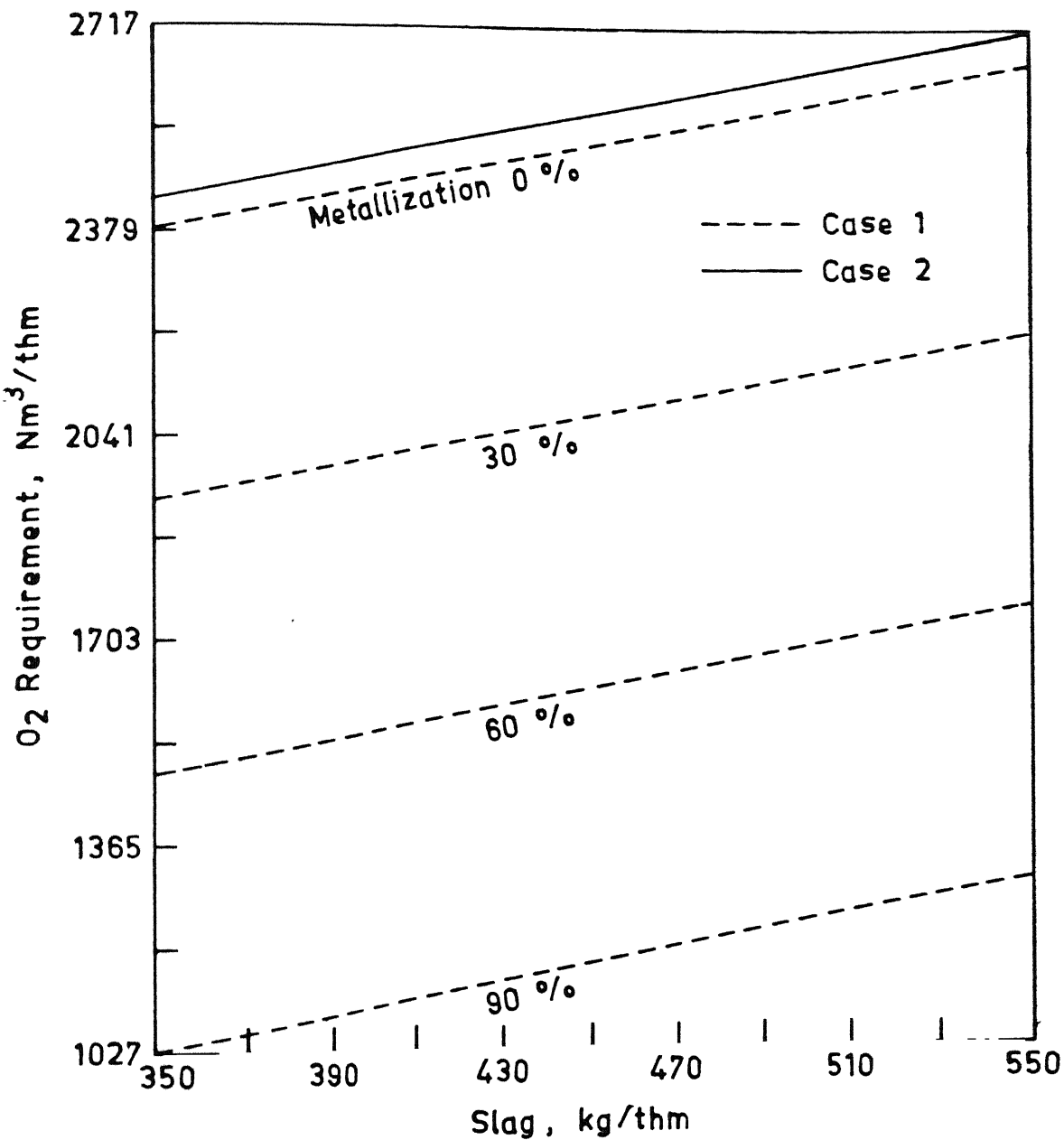


Fig. 4.14 O₂ requirement for coal combustion vs slag amount at various degrees of metallization for both cases

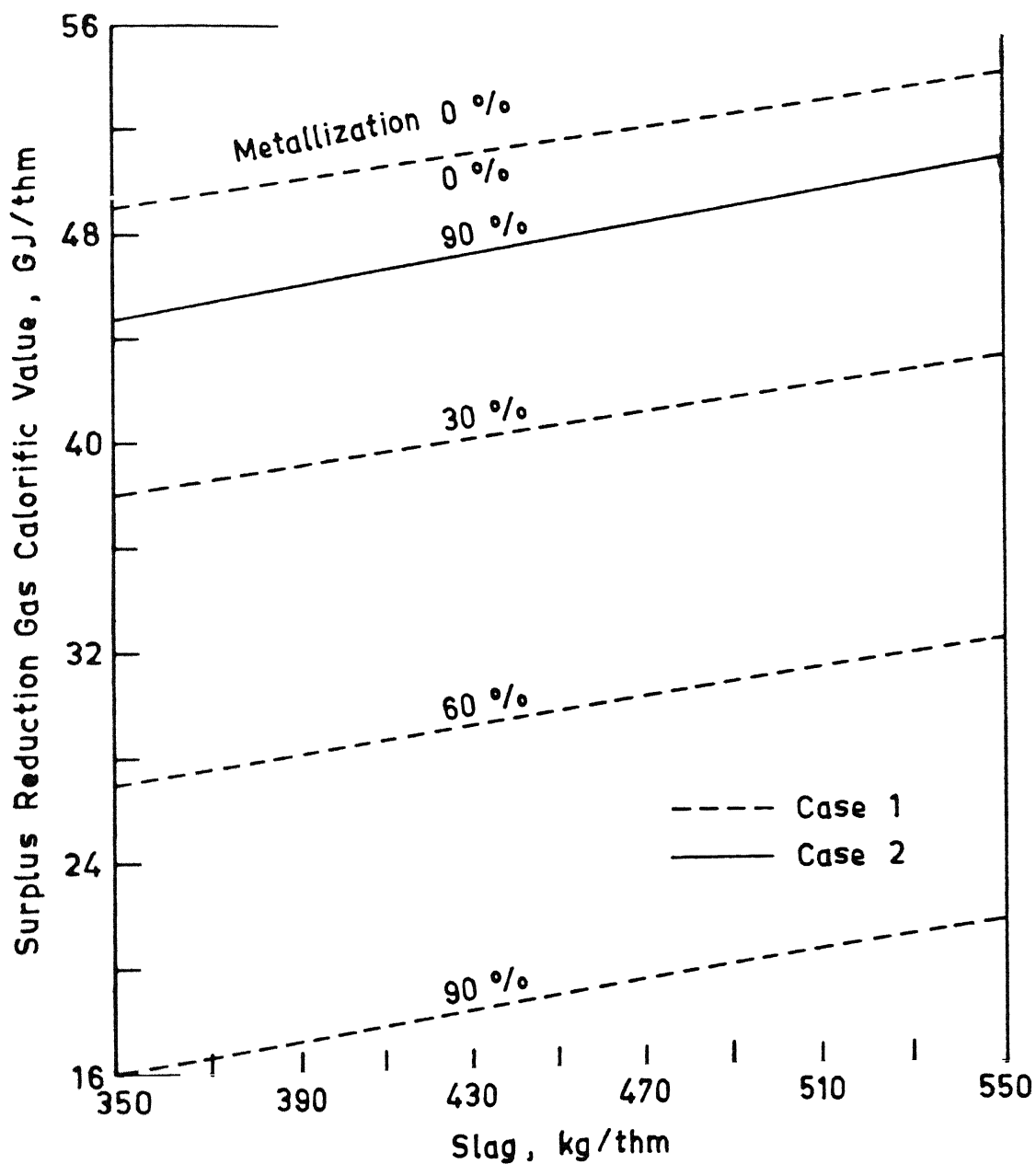


Fig. 4.15 Surplus reduction gas calorific value vs. slag amount at various degrees of metallization for both cases

In the calculations, amount and composition of gangue content of ore, amount of ash and amount of CaCO_3 all together contribute to the increase in slag amount whose materials balances are presented in Table 4.15 and 4.16.

Increased amount of slag requires more heat for decomposition of higher amount of CaCO_3 and raising the temperature of the oxides to the temperature of the slag. So, as the slag amount increases, the heat demand for both the cases increases. This results in increase in coal consumption with the increase in slag amount. This hypothesis is verified by Fig. 4.13 for both cases at various degrees of metallization.

For case 1, at 0% metallization in RSF the coal rate corresponding to slag rate 350, 450 and 550 kg/thm are 1733.92, 1820.71 and 1907.49 kg/thm respectively (see Table 4.2) whereas at 90% metallization in RSF the coal rate corresponding to slag rate 350, 450 and 550 kg/thm are 764.26, 851.04 and 937.83 kg/thm respectively. Similar trend is observed for case 2 and other degrees of metallization.

Corresponding increase in O_2 requirement is also expected with the increase in slag amount as shown in Fig. 4.14. (See Table 4.4 and 4.13). Similar trend is observed for surplus gas calorific value as shown in Fig. 4.15 (See table 4.8).

4.1.4 Coal Grades

Normally a coal is characterized by its volatile matter content and ash content. Various grades of coal can be seen in appendix (VII). In the plots taken under this sub-head, slag rate = 450 kg/thm and post combustion ratio = 0% has been taken. Compositions of coal have been taken on dry ash free (daf) basis (see appendix IX). As we move from anthracite coal to

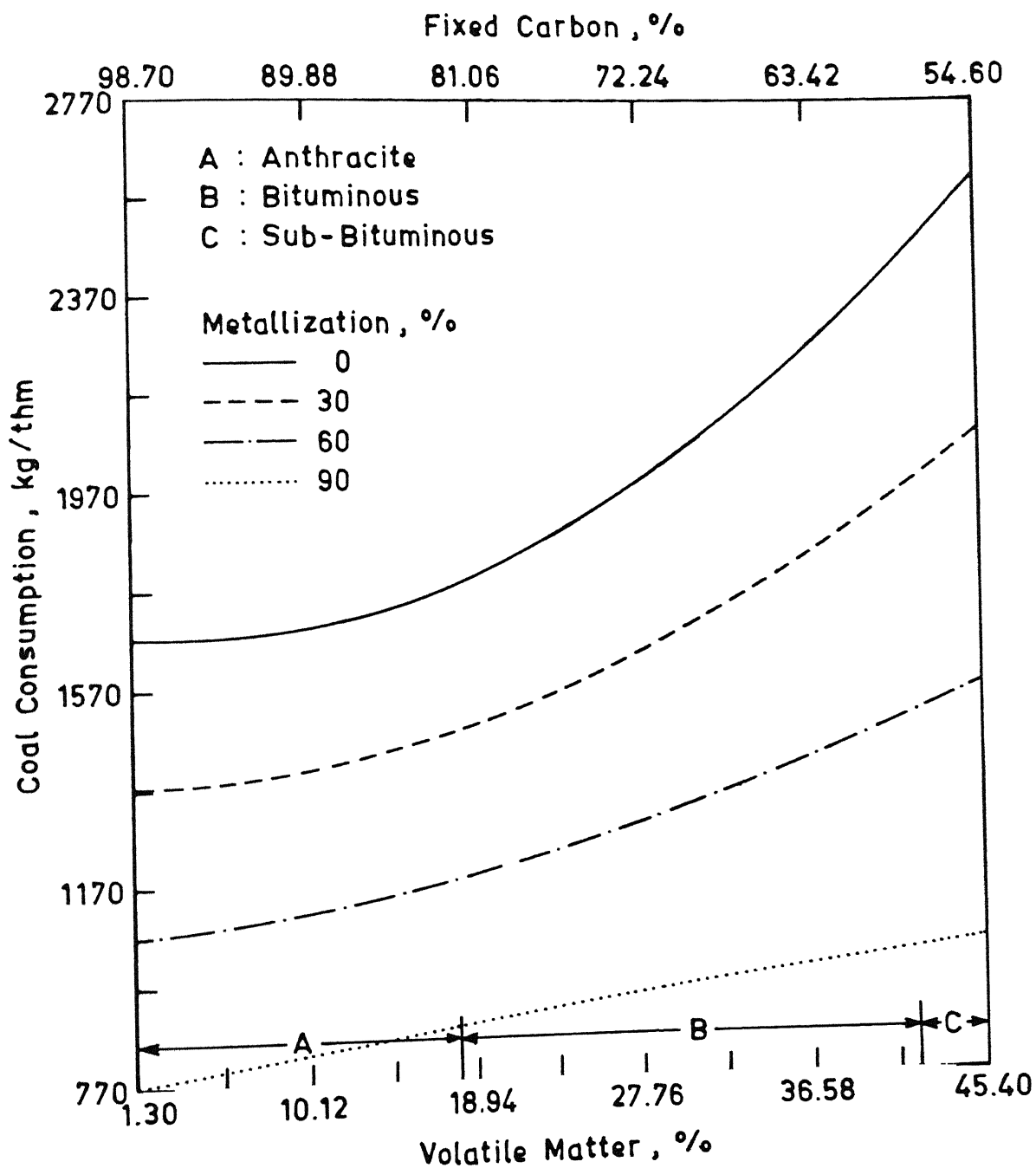


Fig. 4.16 Coal consumption vs coal grade at various degrees of metallization for both cases

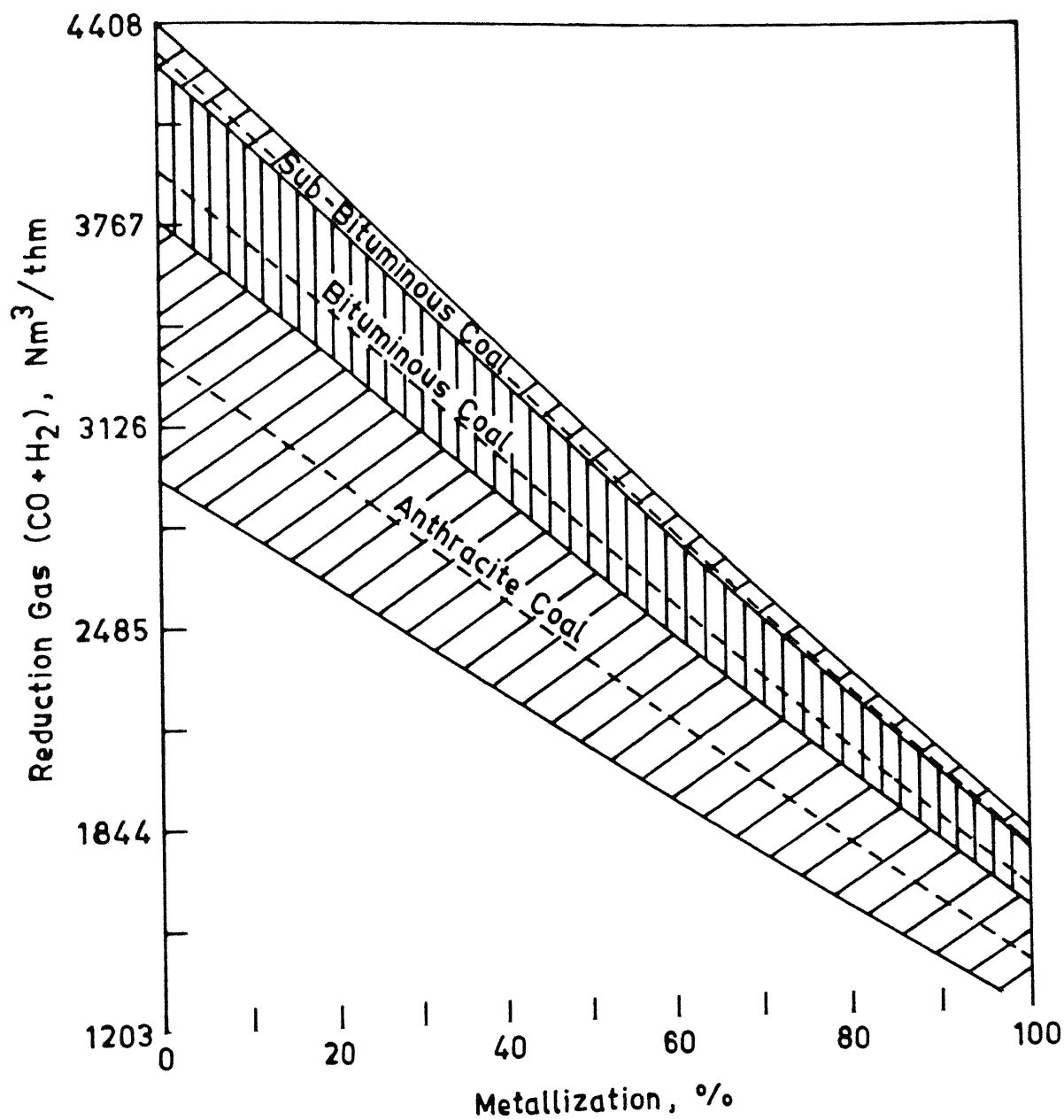


Fig. 4.17 ($\text{CO} + \text{H}_2$) production vs the degree of metallization for various coal grades

sub-bituminous coal, the volatile matter of the coal increases from 1.3 to 45.4%, which also means fixed C of the coal decreases from 98.7 to 54.6%. As fixed C in sub-bituminous coal is less, so more coal will be required to meet the required heat demand. This is evident from Fig. 4.16 which shows coal consumption against volatile matter content and carbon content of coal for various degree of metallization (also see Tables 4.2 and 4.3).

For 0% metallization and case 1, under no post-combustion conditions to meet the thermal and chemical demand of the MG 1646.54 kg/thm of anthracite coal (1.3% VM and 98.7% FC) or 2775.79 kg/thm of sub-bituminous coal (45.4% VM and 54.6% FC) can be used. Several other coals of different amount can also be used to meet the required chemical and thermal demand.

Coal consumption for total heat demand case will be higher than the MG heat demand case as observed earlier. For a particular degree of metallization, sub-bituminous coal which has highest volatile matter will on combustion produces largest amount of reduction gas ($\text{CO} + \text{H}_2$) and anthracite the lowest. The effect of coal grade (sub-bituminous, bituminous and anthracite) on production of ($\text{CO} + \text{H}_2$) in the MG at various degrees of metallization can be seen in Fig. 4.17 and Tables 4.6 and 4.7. Amount of reduction gas ($\text{CO} + \text{H}_2$) produced in the MG is highest in case of sub-bituminous coal ($=4408.78 \text{ Nm}^3/\text{thm}$) because it has high volatile matter content (41 - 46% whereas anthracite coals which have low volatile matter content (1-15%) produce least amount of reduction gas on combustion ($=2966.25 \text{ Nm}^3/\text{thm}$).

In Fig. 4.20 and 4.21, nomograms are constructed to determine the amount of bituminous and sub-bituminous coal consumption in the two stage smelting reduction process. The way to determine

the coal consumption is shown in the figures. For example at 60% metallization, bituminous coal consumption is around 460 kg/thm when slag rate is 350 kg/thm and 20% post combustion is done for the case when only MG thermal and chemical demand is considered.

4.2 BLAST FURNACE PROCESS

Visualization of the blast furnace as two reactors (i.e. the top and bottom segments) is perfectly all right as long as materials and heat balance equations are consistent with continuity of materials and heat between the segments. This division into two parts is done through the chemical reserve zone at 1200 K. So, the thermochemical model developed for the two stage smelting reduction process can be applied to the blast furnace with some modifications. These modifications are presented in appendix VIII where a thermochemical model for blast furnace is developed.

Verification of the model has been done by predicting coke rate for TISCO, VSP and RSP furnaces. This is shown in Fig. 4.18. Table 4.18 shows some data from TISCO blast furnaces. Comparisons between actual and predicted coke rate, top gas temperature and tuyere flame temperature can also be seen. Comparisons for top gas temperature have been plotted in Fig. 4.19.

It is clear from the table and the figures that predicted values match with the actual with sufficient accuracy.

The composition of the top gas as calculated from the model can also be seen in Table 4.18 (plant data for top gas composition and amount is not available).

Table 4.18 Blast furnace data comparison with model values

H O T M E T A L	% Si	0.95	0.96	0.89	0.85	1.16	1.15
	% Mn	0.06	0.06	0.06	0.27	0.36	0.48
	% S	0.58	0.059	0.056	0.06	0.057	0.059
	% C	4.00	4.00	4.00	4.00	4.00	4.00
S L A G	% CaO	32.79	32.91	32.55	32.40	32.69	30.62
	% MgO	8.83	9.90	8.77	9.70	8.69	9.84
	% SiO ₂	34.93	34.70	34.80	34.74	34.52	34.60
	% MnO	0.12	0.12	0.11	0.28	0.35	0.42
	% Al ₂ O ₃	19.95	20.09	20.26	20.39	20.41	20.48
	% CaS	1.02	1.05	1.04	1.06	1.06	1.07
	Rate (kg/thm)	313	308	344	325	290	270
	Blast humidification Nm ³	90.1	88.5	87.8	91.7	89.4	87.2
Blast Temp. (°C)		1076	1050	1038	917	973	964
% C in coke		80.84	75.97	75.65	75.97	75.65	75.97
Coke rate (kg/thm)	A	583	584	614	646	602	654
	P	585.54	588.77	621.59	643.18	653.53	687.25
Top gas temperature (°C)	A	167	162	138	197	224	215
	P	135.98	146.98	171.61	204.52	221.98	268.78
Tuyere flame temperature (°C)	A	1831	1876	1889	1791	1803	1810
	P	1830.97	1818.48	1812.15	1746.92	1755.45	1760.04
Amount of top gas (Nm ³ /thm)		1327.49	1441.34	1517.22	1651.37	1402.63	1533.46
CO/CO ₂ ratio ² in top gas		1.61	1.42	1.48	1.57	1.33	1.42

(A = Actual, P = Predicted by model)

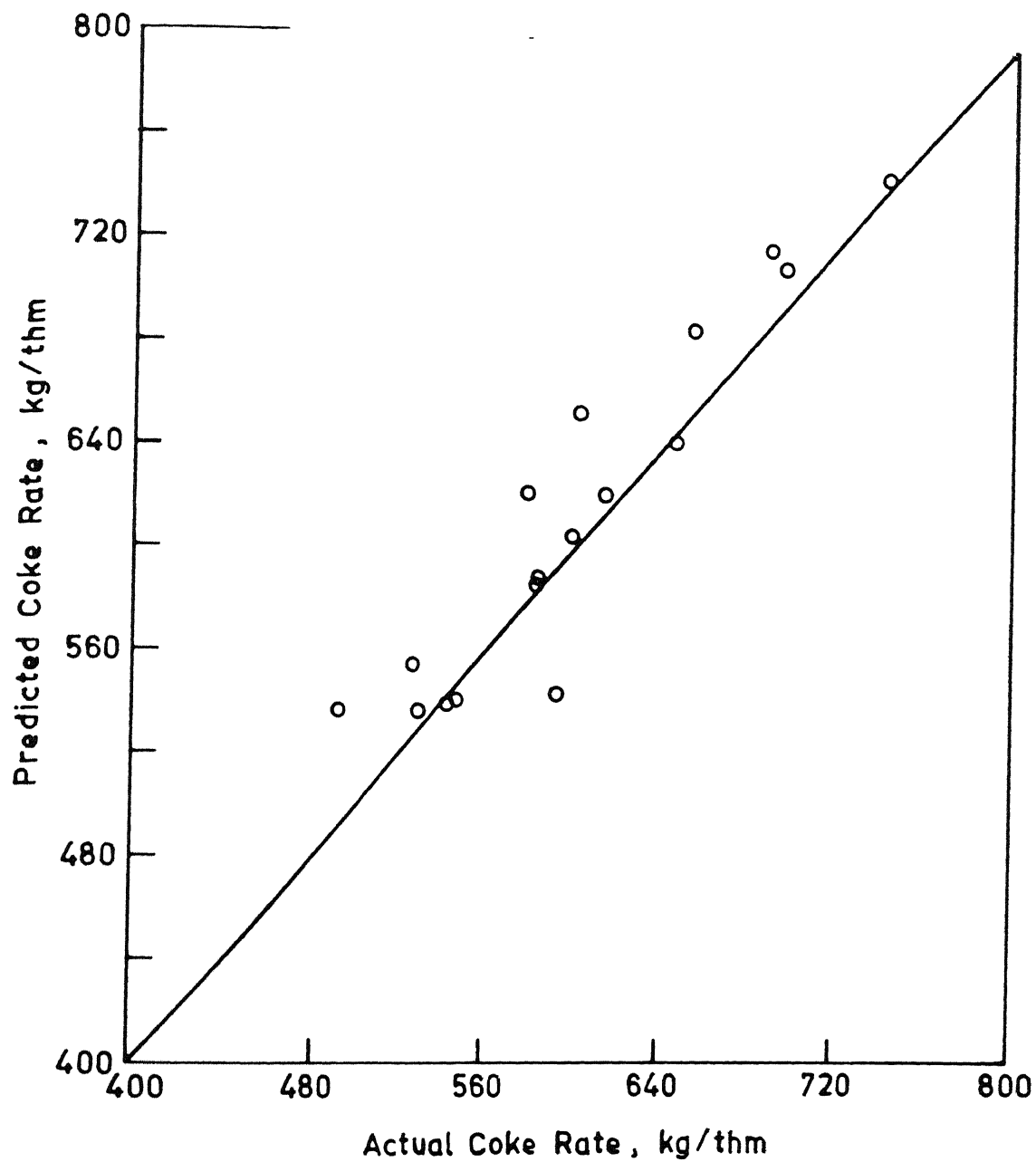


Fig. 4.18 Predicted coke rate vs actual coke rate

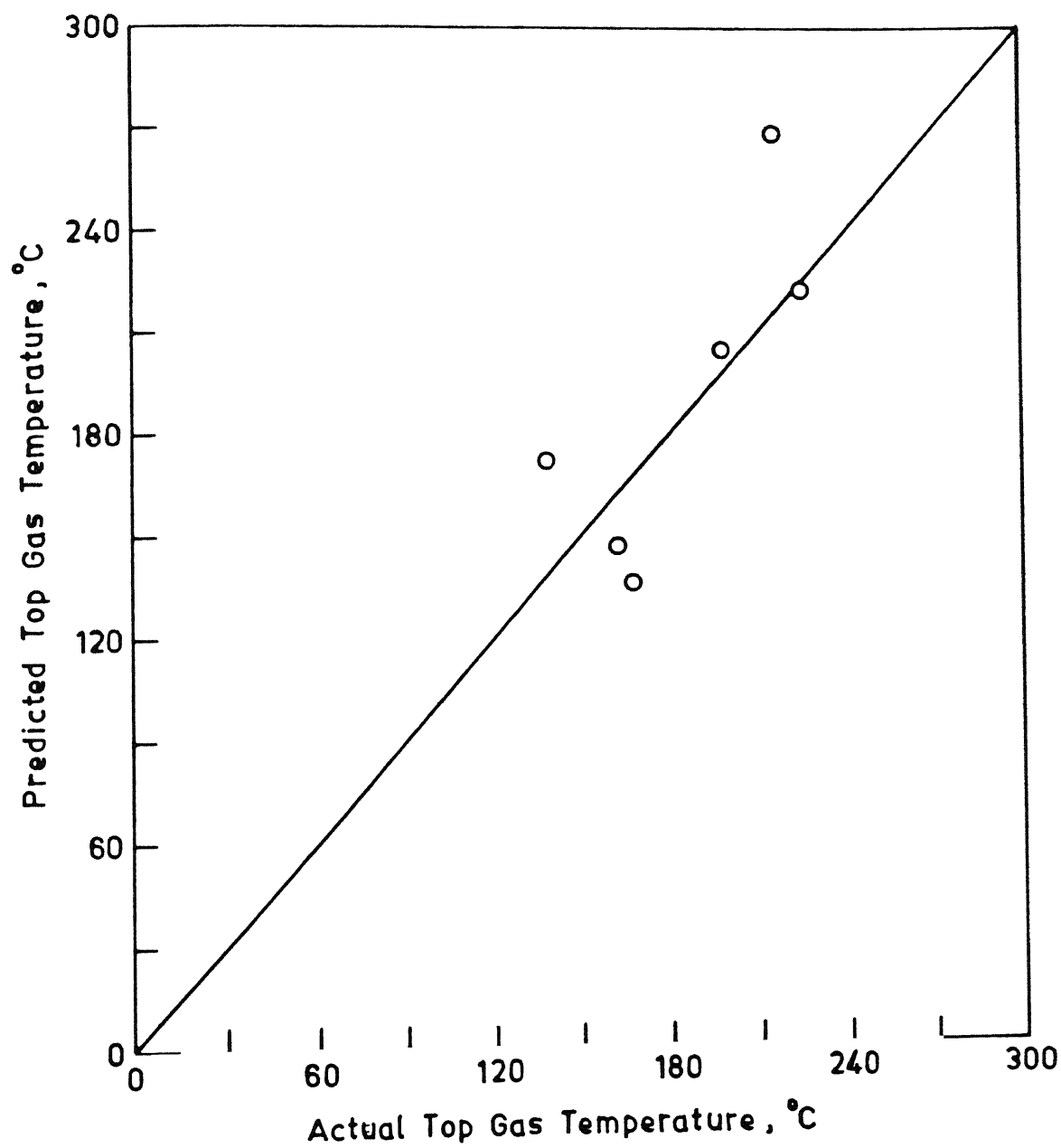


Fig. 4.19 Predicted top gas temperature vs actual top gas temperature

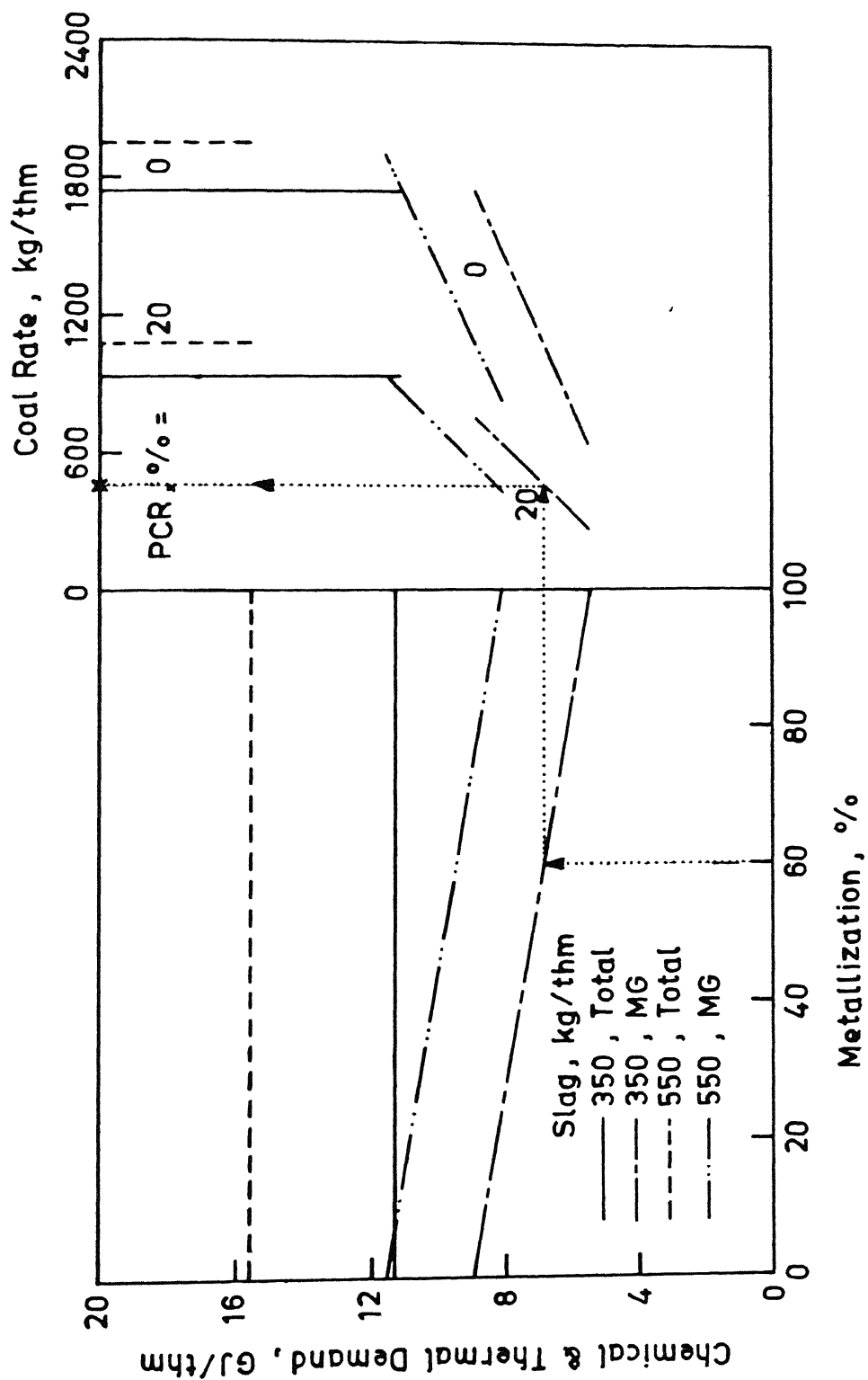


Fig. 4.20 Nomogram for bituminous coal consumption in two stage smelting reduction process

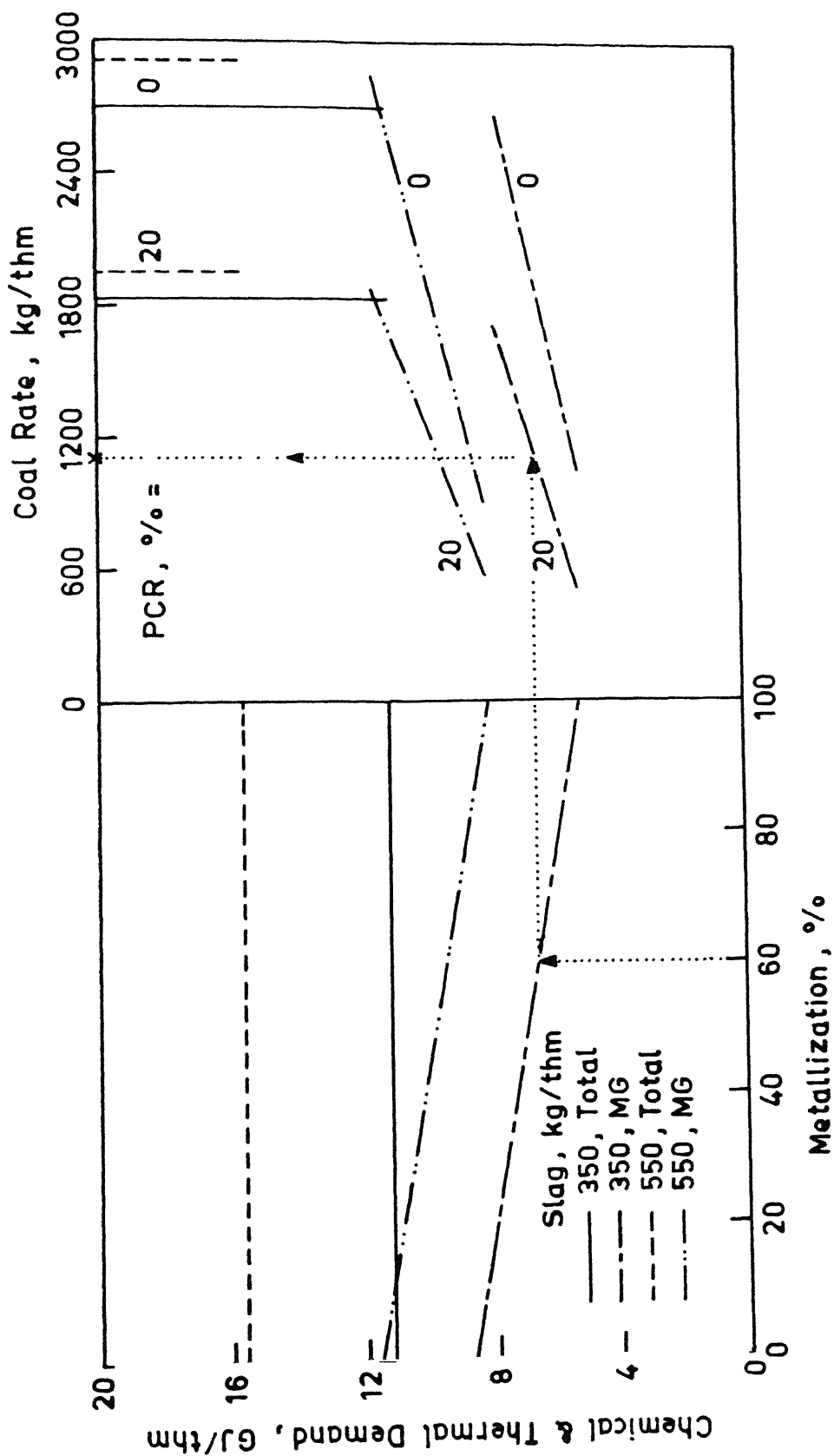


Fig. 4.21 Nomogram for sub-bituminous coal consumption in two stage smelting reduction process

CONCLUSIONS

As a result of the present study, the following conclusions are made:

1. With the availability of plant data for heat and dust losses, the thermo-chemical model developed for the two-stage smelting reduction process can predict coal rate, O_2 requirements, reduction gas and top gas amount and composition and the surplus energy with reasonably good accuracy.
2. The thermo-chemical model modified for the blast furnace also predicts coke rate, O_2 requirement, top gas temperature, amount and its composition, tuyere flame temperature with good accuracy.
3. Coal consumption, O_2 requirement, reduction gas production and surplus energy all decrease with the increase in the degree of metallization in the reduction shaft furnace when only the MG thermal and chemical demand is met by coal combustion. These become minimum at the optimum degree of metallization where no surplus energy is available.
4. When the total chemical and thermal demands for both the reactors (MG and RSF) is considered to be met by coal combustion, above quantities remain constant. The concept of optimum utilization of reduction gas cannot be realized here because very high amount of reduction gas is produced.
5. Post - combustion greatly reduces coal consumption, O_2

requirement, reduction gas production and surplus energy. However, once post-combustion exceeds 30%, the gas loses much of its potential to reduce $\text{Fe}_{0.95}\text{O}$ to Fe in the reduction shaft furnace. So, CO_2 and H_2O scrubbing becomes necessary above 30% post-combustion.

6. Higher amount of slag requires more coal to be combusted which in turn results in higher O_2 requirement, reduction gas production and surplus energy.
7. Two-stage smelting reduction process is not restricted to a particular variety of coal. Anthracite coal consumption to meet a particular thermal and chemical demand is lower than other grades of coal (bituminous and sub-bituminous). Sub-bituminous coals because of their highest volatile matter content give highest amount of reduction gas among anthracite, bituminous and sub-bituminous coals.
8. Since only that much amount of scrubbed reduction gas (i.e. $\text{CO} + \text{H}_2$) is sent to the RSF which is required for pre-reduction of wustite to iron, the top gas composition and amount remains fixed for a particular degree of metallization.

CHAPTER - 6

SUGGESTIONS FOR FURTHER WORK

Following suggestions are made for further work:

1. In the present study, the losses of heat and material in scrubbers, hot gas cyclone and during transfer from one reactor to the other are not considered. Energy requirement for scrubbing has also not been included in the work. A thermo-chemical model for the overall process (COREX process) can be developed by incorporating above information in the model developed for two stage smelting reduction process.
2. During the post-combustion of the reducing gases, the flame temperature may reach a value which is unsuitable for the furnace lining. A separate post-combustion model can be made which calculates the optimum degree of post-combustion for a given set of conditions.

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APPENDIX I

Enthalpies of formation at temperature T from elements at temperature T

(H_T^f) [21]

Values are accurate to within ± 500 KJ.

Compound	Units : KJ per kg mole of compound			
	298K	1100 K	1200 K	1300 K
CH ₄	-75000	-91000	-91000	-92000
C ₂ H ₆	-84000	-102000	-101000	-100000
C ₃ H ₈	-105000	-129000	-128000	-127000
CO	-111000	-113000	-113000	-114000
CO ₂	-394000	-395000	-395000	-395000
CaCO ₃ (from CaO, C & O ₂)	-572000	-563000	-561000	-559000
CaCO ₃ .MgCO ₃ (from carbonates)	-12000	decomposes below 1100 K		
CaCO ₃ P ₂ O ₅ (from CaO, O ₂ & P _{3g})	-2400000	-2364000	-2353000	-2341000
CaO.SiO ₃ (from oxides)	-89000	-91000	-91000	-91000
(CaO) ₃ .SiO ₃ (from oxides)	-126000	-125000	-124000	-123000
P ₂ O ₅			-1554000	
Fe _{0.947} O	-266000	-265000	-265000	-265000
Fe ₃ O ₄	-1121000	-1096000	-1098000	-1095000
Fe ₂ O ₃	-826000	-810000	-811000	-809000
H ₂ O _l ($\Delta H_{298}^{\text{Vaporization}} = + 44000$)	-286000			
H ₂ O _g	-242000	-248000	-249000	-250000 (also -250000 at 1500K)
MgCO ₃ (from MgO, C & O ₂)	-511000	decomposes below 1100K		
MnO	-385000	-386000	-386000	-386000
Mn ₃ O ₄	-1387000	-1387000	-1386000	-1384000
MnO ₂	-521000	-516000	decomposes at 1120K	
SO ₂ (from gaseous S ₂)	-362000	-362000	-362000	-362000
SiO ₂	-911000	-902000	-901000	-901000

APPENDIX II

Enthalpy Increment Equations for Elements and Compounds $\left[H_T^0 - H_{298}^0 \right]$

Enthalpy values calculated with these equations are within $\pm 500\text{kJ}$ of their published numerical equivalents [21].

Substance	Units: kJ per kg mole of element or compound				
	Temperature range, K				
	298-800 Top gas	800-1100	1100-1300 Wustite reduction	1100 -1900 Bosh & Hearth	1800-2800 Flame Tem
Al_2O_3	107T-32000	124T-46000	128T-50000	132T-55000	-
C	15.3T-4600	20.7T-8700	22.7T-11000	13.5T-11800	-
CO	30.2T-9100	32.5T-10800	34.2T-12600	35.3T-14000	36.6T-164
CO_2	45.6T-14100	52.8T-19200	56.3T-23100	58.6T-26000	61.0T-305
CaO	48.5T-14500	51.6T-17000	54.2T-19800	55.5T-21200	-
CaCO_3	106T-31500	123T-45100	129T-52200	Decomposes above 1300k	
$\text{CaO} \cdot \text{SiO}_2$	108T-32300	122T-43600	128T-49500	128T-50000	-
$(\text{CaO})_2 \cdot \text{SiO}_2$	158T-47000	186T-69000	189T-73000	218T-105000	-
$(\text{CaO})_3 \cdot \text{P}_2\text{O}_5$	284T-84500	356T-142000	402T-193000	403T-194000	-
Fe_S	30.8T-9200	48.9T-23700	-	38.4T-11400	-
Fe_l (MP \approx 1800K)	-	-	-	44.0T-5800	-
$\text{Fe}_{0.947}\text{O}$	52.2T-15600	56.4T-18900	58.6T-21400	61.1T-24100	-
Fe_2O_3	135t-40200	158T-58800	142T-40600	144T-43000	-
Fe_3O_4	202T-60000	227T-82000	201T-53200	201T-53200	-
H_2	29.3T-8800	29.9T-9200	30.9T-10300	32.5T-12200	35.2T-172
$\text{H}_2\text{O}(\text{g})$	35.8T-10800	40.0T-13800	43.7T-17900	47.4T-22200	-
MgO	45.6T-13600	50.9T-17800	52.2T-19300	55.0T-22300	-
MgCO_3	102T-30500	126T-49500	Decomposes below 1100K		-
Mn_S	31.0T-9200	44.3T-19900	38.2T-13200	48.6T-24600	-
Mn_l (MP=1517K)	-	-	-	48.6T-10000	-
MnO	49.2T-14700	53.7T-18300	56.9T-21800	57.1T-22000	-
MnO_3	68.2T-20300	77.3T-27600	-	-	-
Mn_3O_4	167T-49600	182T-61900	199T-80200	238T-123000	-
N_2	30.0T-9000	32.1T-10500	-	34.4T-13000	36.4T-165
O_2	31.6T-9600	34.3T-11500	-	36.2T-13500	-
$\text{P}_{2\text{g}}$	34.9T-10500	36.7T-11900	37.2T-12300	37.1T-13600	-
$\text{S}_{2\text{g}}$	35.2T-10600	36.9T-11900	37.2T-12300	37.4T-12500	-
Si_S	23.6T-7000	26.4T-9300	27.2T-10200	27.1T-10100	-
Si_l (MP=1683K)	-	-	-	27.2T+40400	-
SiO_2	61.1T-18200	71.0T-25900	71.4T-24300	72.8T-26200	-

APPENDIX III

Calculation of model variables in terms of kg mole of the component/kg mole of the product iron.

$$C/Fe = \frac{(\% C \text{ in HM})}{12} \frac{56}{(\% Fe \text{ in HM})}$$

$$Si/Fe = \frac{(\% Si \text{ in HM})}{28} \frac{56}{(\% Fe \text{ in HM})}$$

$$Mn/Fe = \frac{(\% Mn \text{ in HM})}{55} \frac{56}{(\% Fe \text{ in HM})}$$

$$S/Fe = \frac{(\% S \text{ in HM})}{32} \frac{56}{(\% Fe \text{ in HM})}$$

$$P/Fe = \frac{(\% P \text{ in HM})}{31} \frac{56}{(\% Fe \text{ in HM})}$$

Slag in kg/kg mole of produced Fe (W_{slag})

$$= \frac{Slag \text{ (kg/thm)}}{1000} \times \frac{56}{1} \times \frac{100}{\% Fe}$$

$$= \frac{Slag \text{ (kg/thm)} \times 5.6}{(\% Fe \text{ in HM})}$$

$$n_{CaO} = \frac{(\% CaO \text{ in slag}) \times W_{slag}}{100 \times 56.1}$$

$$n_{SiO_2} = \frac{(\% SiO_2 \text{ in slag}) \times W_{slag}}{100 \times 60}$$

$$n_{Al_2O_3} = \frac{(\% Al_2O_3 \text{ in slag}) \times W_{slag}}{100 \times 102}$$

$$n_{MnO} = \frac{(\% MnO \text{ in slag}) \times W_{slag}}{100 \times 70.9}$$

$$n_{CaS} = \frac{(\% CaS \text{ in slag}) \times W_{slag}}{100 \times 72}$$

APPENDIX IV

Calculation of components of reduction gas

n_C^A kg moles of C per kg mole of Fe react with oxygen in the melter-gasifier to produce CO.

Total kg moles of CO produced per kg mole of Fe = n_C^A

Total kg moles of H_2 formed per kg mole Fe = $n_{H_2}^O$

If some percentage of above gases (=ppc) is post-combusted in the melter-gasifier to give CO_2 and H_2O , then kg moles of above gases participating in post-combustion per kg mole of Fe are given by

$$\frac{\text{kg moles of } CO_2 \text{ in reduction gas per kg mole Fe}}{(n_{CO_2}^r)} = n_C^A \cdot \frac{ppc}{100}$$

(n_C^A is taken from equation 3.9)

$$\frac{\text{kg moles of } H_2O \text{ in reduction gas per kg mole of Fe}}{(n_{H_2O}^r)} = \frac{n_{H_2}^O}{2} \cdot \frac{ppc}{100}$$

($n_{H_2}^O$ is taken from equation 3.32)

$$\frac{\text{Remaining kg moles of CO in the reduction gas per kg mole of Fe}}{(n_{CO}^r)} = n_C^A \left(1 - \frac{ppc}{100}\right)$$

$$\frac{\text{Remaining kg moles of } H_2 \text{ in the reduction gas per kg mole of Fe}}{(n_{H_2}^r)} = \frac{n_{H_2}^O}{2} \left(1 - \frac{ppc}{100}\right)$$

$$\frac{\text{kg moles of } N_2 \text{ in the reduction gas per kg mole Fe}}{(n_{N_2}^r)} = \frac{C_X \left(\% N \text{ in coal}\right)}{2 \times 14 \times 100}$$

$$\text{Total reduction gas } (n_t^r) = n_{CO_2}^r + n_{CO}^r + n_{H_2}^r + n_{H_2O}^r + n_{N_2}^r$$

So, percentage of CO in the reduction gas $\left(p_{CO}^r\right) = \frac{n_{CO}^r}{n_t^r} \times 100$

So composition of reduction gas leaving MG is $p_{CO}^r, p_{CO_2}^r, p_{H_2}^r, p_{H_2O}^r, p_{N_2}^r$

If n_t^{ro} is the total kg moles of the reduction gas as taken out of the process then,

$$n_{CO}^{ro} = n_t^{ro} = \frac{p_{CO}^r}{100}$$

Similarly $n_t^{ro}, n_{H_2}^{ro}, n_{H_2O}^{ro}, n_{N_2}^{ro}$ can be calculated.

Now $\left(n_{CO}^r - n_{CO}^{ro}\right), \left(n_{CO_2}^r - n_{CO_2}^{ro}\right), \left(n_{H_2}^r - n_{H_2}^{ro}\right), \left(n_{H_2O}^r - n_{H_2O}^{ro}\right)$ and $\left(n_{N_2}^r - n_{N_2}^{ro}\right)$ are the components of the reduction gas going in the reduction shaft furnace.

$$\text{Now } n_{CO}^{req} = \left(\frac{X}{100}\right) \frac{\left[3.3 - 1.22\left(n_{H_2}^r\right)''\right]}{0.95}$$

(kg moles of CO required in the reduction shaft per kg mole Fe)

$$\text{and } n_{H_2}^{req} = \left(\frac{X}{100}\right) \frac{\left(n_{H_2}^r\right)''}{0.95}$$

Also utilization of CO and H_2 at 1200 K for $Fe_{0.95}O - Fe$ equilibrium is 30% and 37% respectively.

So, top gas will have following kg mole of components per kg mole of product Fe.

$$n_{CO}^{tg} = \left(n_{CO}^r - n_{CO}^{ro}\right) - n_{CO}^{req} + \frac{2.3}{3.3} n_{CO}^{req}$$

$$n_{H_2}^{tg} = \left(n_{H_2}^r - n_{H_2}^{ro}\right) - n_{H_2}^{req} + \frac{1.7}{2.7} n_{H_2}^{req}$$

$$n_{N_2}^{tg} = \left(n_{N_2}^r - n_{N_2}^{ro}\right)$$

$$n_{H_2O}^{tg} = \left(n_{H_2O}^r - n_{H_2O}^{ro}\right) + \frac{1}{2.7} n_{H_2}^{req}$$

$$n_{CO_2}^{tg} = \left(n_{CO_2}^r - n_{CO_2}^{ro}\right) + \frac{1}{3.3} n_{CO}^{req}$$

Also

$$\left(\text{O/C}\right)^{\text{tg}} = \frac{n_{\text{CO}}^{\text{tg}} + 2 n_{\text{CO}_2}^{\text{tg}}}{n_{\text{CO}}^{\text{tg}} + n_{\text{CO}_2}^{\text{tg}}}$$

$$\left(\text{O/H}_2\right)^{\text{tg}} = \frac{n_{\text{H}_2\text{O}}^{\text{tg}}}{n_{\text{H}_2}^{\text{tg}} + n_{\text{H}_2\text{O}}^{\text{tg}}}$$

Similarly,

$$\left(\text{O/C}\right)^{\text{rg}} = \frac{n_{\text{CO}}^{\text{rg}} + 2 n_{\text{CO}_2}^{\text{rg}}}{n_{\text{CO}}^{\text{rg}} + n_{\text{CO}_2}^{\text{rg}}}$$

$$\left(\text{O/H}_2\right)^{\text{rg}} = \frac{n_{\text{H}_2\text{O}}^{\text{rg}}}{n_{\text{H}_2}^{\text{rg}} + n_{\text{H}_2\text{O}}^{\text{rg}}}$$

APPENDIX V

Calculation of n_{Si}^a , $n_{SiO_2}^b$, n_{Si}^c and $n_{SiO_2}^d$

n_{Si}^a = kg moles of SiO_2 from ore per kg mole of Fe (joining HM as Si)

$n_{SiO_2}^b$ = kg moles of SiO_2 from ore per kg mole of Fe (joining slag as SiO_2)

n_{Si}^c = kg moles of SiO_2 from ash of coal per kg mole of Fe (joining HM as Si)

$n_{SiO_2}^d$ = kg moles of SiO_2 from coal per kg mole of Fe (joining slag as SiO_2)

$$\text{Let } \frac{n_{Si}^a}{n_{SiO_2}^b} = \alpha$$

$$\text{and } \frac{n_{Si}^c}{n_{SiO_2}^d} = \beta \text{ and } n_{Si}^a + n_{SiO_2}^b = n_{SiO_2}^{\text{ore}}$$

$$\text{So, } n_{Si}^a = \frac{\alpha}{\alpha + 1} \cdot n_{SiO_2}^{\text{ore}}$$

$$n_{SiO_2}^b = \frac{1}{\alpha + 1} \cdot n_{SiO_2}^{\text{ore}}$$

$$\left(n_{SiO_2}^{\text{ore}} \text{ is known from equation 3.19} \right)$$

Also,

$$n_{Si}^c = \frac{\beta}{(\beta + 1)} n_{SiO_2}^{\text{coal}}$$

$$n_{SiO_2}^d = \frac{1}{(\beta + 1)} \cdot n_{SiO_2}^{\text{coal}}$$

$$\left(n_{SiO_2}^{\text{coal}} \text{ is known from equation 3.16} \right)$$

Calculation of n_S^a , n_{CaS}^b , n_S^c and n_{CaS}^d

n_S^a = kg moles of S from ore per kg mole of Fe (joining HM as S)

n_{CaS}^b = kg moles of S from ore per kg mole of Fe (joining slag as CaS)

n_S^c = kg moles of S from ash of coal per kg mole of Fe (joining HM as S)

$n_{\text{CaS}}^{\text{d}}$ = kg moles of S from coal per kg mole of Fe (joining slag as S)

$$\text{Let } \frac{n_{\text{S}}^{\text{a}}}{n_{\text{CaS}}^{\text{b}}} = \gamma$$

$$\text{and } \frac{n_{\text{S}}^{\text{c}}}{n_{\text{CaS}}^{\text{d}}} = \delta$$

$$\text{So, } n_{\text{S}}^{\text{a}} = \frac{\gamma}{\gamma + 1} \cdot n_{\text{FeS}}^{\text{ore}}$$

$$n_{\text{CaS}}^{\text{b}} = \frac{1}{\gamma + 1} \cdot n_{\text{FeS}}^{\text{ore}}$$

$(n_{\text{FeS}}^{\text{ore}}$ is known from equation 3.27)

Also,

$$n_{\text{S}}^{\text{c}} = \frac{\delta}{(\delta + 1)} n_{\text{FeS}}^{\text{coal}}$$

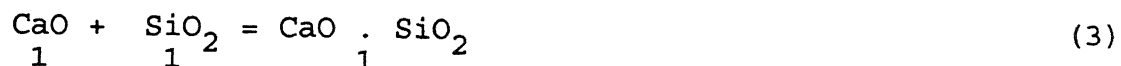
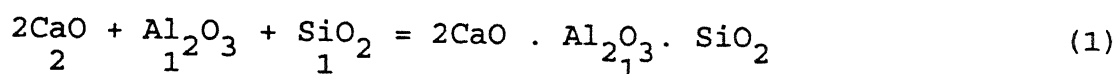
$$n_{\text{CaS}}^{\text{d}} = \frac{1}{(\delta + 1)} \cdot n_{\text{S}}^{\text{coal}}$$

$(n_{\text{S}}^{\text{coal}}$ is known from equation 3.24)

APPENDIX VI

Heat of Slag Formation

Reactions occurring in the slag are :



RC	MnO	MgO	CaO	Al ₂ O ₃	SiO ₂	CaS	(All per kg mole Fe)
1			2	(1)	1		Number of kg moles of 2CaO.Al ₂ O ₃ .SiO ₂ = kg moles of Al ₂ O ₃ (n _{Al₂O₃})
2			2		1		
3			1		1		
4	(1)				1		kg moles of MnO.SiO ₂ = kg moles of MnO (n _{MnO})
5						(1)	Number of kg moles of CaS = kg moles of CaS (n _{CaS})
6		(2)			1		kg moles of 2MgO.SiO ₂ = 2 (kg moles of MgO) = 2 n _{MgO}

Let moles of 2CaO.SiO₂ = p

and moles of CaO .SiO₂ = q

From reactions (2) and (3)

kg moles of CaO left for reaction (2) and (3) per kg mole of

$$\text{Fe} = 2p + q$$

$$= \left(n_{\text{CaO}} - 2 n_{\text{Al}_2\text{O}_3} \right) = r$$

kg moles of SiO₂ left for reactions (2) and (3) per kg mole of

$$\text{Fe} = p + q$$

$$= \left(n_{\text{SiO}_2} - n_{\text{Al}_2\text{O}_3} - n_{\text{MnO}} - 0.5 n_{\text{MgO}} \right) = s$$

$$2p + q = r$$

$$-(p + q = s)$$

$$p = r - s$$

$$q = s - p$$

d_{slag} = heat released in slag formation per kg mole of product Fe

$$= - \left[q.90300 + p.126840 \right] + n_{\text{Al}_2\text{O}_3}.104580 + n_{\text{MnO}}.24780 + 2 n_{\text{MgO}}.63420 + n_{\text{CaS}}.0$$

APPENDIX VII

Typical compositions of coals of different grades (dry basis)

Group (ASTM designation D388)	Ultimate analyses (%)					
	Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur	Ash
Metaanthracite	86.8	1.6	2.0	0.6	0.9	8.1
Anthracite	84.2	2.8	2.2	0.8	0.6	9.4
Semianthracite	78.3	3.6	2.3	1.4	2.0	12.4
Bituminous						
Low volatile	85.4	4.8	2.6	1.5	0.8	4.9
Medium volatile	86.4	4.9	3.6	1.6	0.6	2.9
High volatile A	79.5	5.2	6.1	1.4	1.3	6.5
High volatile B	78.3	5.2	8.2	1.5	1.4	5.4
High volatile C	73.1	4.8	8.9	1.5	2.6	9.1
Subbituminous						
A	75.1	5.0	12.8	1.4	1.0	4.70
B	75.0	4.9	15.5	1.3	0.5	2.80
C	64.2	4.4	16.6	1.2	0.4	13.2

APPENDIX VIII

Modifications in the developed thermo-chemical model to make it applicable to the blast furnace.

Visualization of the blast furnace as two reactors (i.e. top and the bottom segments) is perfectly all right as long as materials and heat balance equations are consistent with continuity of materials and heat between the segments. This division into two parts is done through the chemical reserve zone at 1200K.

With some modifications the model developed for two stage smelting reduction process can be applied to the blast furnace. Bottom segment of the divided blast furnace is called 'Wustite Reduction Zone' (WRZ).

Following modifications are to be incorporated -

- (1) Gas leaving the WRZ has following equilibrium concentration:
$$\left(\text{O/C}\right)^{\text{WRZ}} = 1.3 \text{ and } \left(\text{O/H}_2\right)^{\text{WRZ}} = 0.37$$
- (2) Instead of pure oxygen, preheated air blast is used here in which injectants (moisture, O_2 and hydrocarbons) may be incorporated.
- (3) Instead of coal combustion, combustion of coke takes place here in which volatile matter is missing. Coke enters WRZ at 1200K.
- (4) The only gas coming out of the process is the top gas here.
- (5) No cooling of gas takes place in blast furnace process.
- (6) No post-combustion of the gas is carried out in the blast furnace.
- (7) In blast furnace MgCO_3 is also used in the flux.
- (8) In blast furnace some scrap may also be charged. So, O/Fe of the iron containing burden going into the WRZ

$$= 1.05 - \left(\frac{1.05 \times 56}{1000} \text{ (kg moles of scrap/thm)} \right)$$

Fully predictive model for blast furnace can be developed, if materials and heat balance is applied to WRZ because (O/Fe), (O/C)^{WRZ}, (O/H₂)^{WRZ}, (O/H₂)^{WRZ} and the temperature of gases leaving WRZ are known. So, the equation for the carbon balance (3.9) changes to,

$$n_C^A = n_C^{\text{coke}} + n_{\text{CaCO}_3} + x n_{\text{inj}} - (\text{C/Fe}) \quad (\text{a})$$

where n_C^{coke} = kg moles of C in coke per kg mole of Fe

n_{inj} = kg moles of injectant ($C_x(H_2)_yO_z$) per kg mole of Fe

The equations for oxygen balance (3.42) modifies to,

$$n_O^B = 1.3 n_C^A + 0.37 Y n_{\text{inj}} - 1.05 + \left[\frac{1.05}{17.9} \left(\text{kg moles of scrap/thm} \right) \right] \\ - 2 (\text{Si/Fe}) - (\text{Mn/Fe}) - 2.5 (\text{P/Fe}) - n_{\text{CaCO}_3} \quad (\text{b})$$

(One kg mole of $C_x(H_2)_yO_z$ gives Y kg mole of H₂ on decomposition)

And equation for heat demand for WRZ comes with the slight modification to equation (3.53).

$$\left(\begin{array}{c} \text{Heat demand} \\ \text{for WRZ} \end{array} \right) = \left(\begin{array}{c} \text{Hot metal} \\ \text{Heat demand} \end{array} \right) + \left(\begin{array}{c} \text{Slag heat} \\ \text{demand} \end{array} \right) \\ + \left(\begin{array}{c} \text{Heat absorbed} \\ \text{by endothermic} \\ \text{reactions} \end{array} \right) + \text{Heat Losses} \quad (\text{c})$$

Since the reference temperature has been taken as 1200 K for heat demand and supply, there is no need to consider the sensible heat loss by gases leaving WRZ at 1200K. MgCO₃ decomposition occurs in the top portion of the blast furnace, so it does not affect WRZ heat demand. MgO is considered in the slag, so $n_{\text{MgO}}[55(T_M - 1200)]$ term gets added to the sensible heat of the slag. Heat for following reaction is also considered in the slag formation : $2\text{MgO} + \text{SiO}_2 = 2\text{MgO}.\text{SiO}_2$ (given in Appendix VI). There is no need to consider n_{Si}^a , $n_{\text{SiO}_2}^b$, n_{Si}^c , $n_{\text{SiO}_2}^d$, n_{S}^a , n_{CaS}^b , n_{S}^c and

n_{CaS}^d here because both coke and pre-reduced ore enter WRZ at the same temperature, Si/Fe and S/Fe will suffice.

Equation for heat supply consists of combustion of C to CO and CO₂ and H₂ to H₂O plus the sensible heat of the air blast coming at T_B^O K.

$$\begin{aligned}
 \text{Heat supply} &= - n_C^A \left[\left\{ 2 - \left(O/C \right)^{WRZ} \right\} \left(-H_{CO}^f \right) \right. \\
 &\quad + \left. \left\{ \left(O/C \right)^{WRZ} - 1 \right\} \left(-H_{CO_2}^f \right) \right] - 0.37 Y n_{inj} \left(-H_{H_2O}^f \right) \\
 &\quad + \left[\left(\frac{1}{2} H_{O_2}^O - \frac{1}{2} H_{O_2}^O \right) + \frac{0.79}{0.21} \left(\frac{1}{2} H_{N_2}^O - \frac{1}{2} H_{N_2}^O \right) \right] n_O^B \\
 &= n_C^A (198000) + Y n_{inj} (92130) + E_B \cdot n_O^B \quad (d)
 \end{aligned}$$

Coupled heat and materials balance equation thus becomes

$$\begin{aligned}
 D_{WRZ} &= n_C^A \left(198000 + 1.3 E_B \right) \\
 &\quad - E_B \left\{ 1.05 - \frac{1.05}{17.9} \left(\text{kg moles of scrap/thm} \right) + Z n_{inj} \right. \\
 &\quad + 2(Si/Fe) + (Mn/Fe) \\
 &\quad \left. + 2 n_{CaCO_3} \right\} + 0.37 Y n_{inj} (249000 + E_B) \quad (e)
 \end{aligned}$$

In above equation the only unknown is n_C^A so its value when substituted in equation (a) gives the coke rate i.e. n_C^{coke} . To know the air requirement n_C^A is substituted in equation (b), which gives us the value of n_O^B .

n_C^A and n_O^B being known now which are valid for the overall furnace, we can carry out overall heat and materials balance for the entire blast furnace to get the value of top gas temperature and composition. Corresponding equations used in the model are:

$$n_O^B + \left(O/C\right)^{tg} + z \cdot n_{inj} + 2 \left(Si/Fe\right) + \left(Mn/Fe\right) + 2.5 \left(P/Fe\right) + 2 n_{CaCO_3} + 2 n_{MgCO_3} = \left(O/C\right)^{tg} n_C^A + Y n_{inj} \left(O/H_2\right)^{tg} \quad (f)$$

$$\frac{\left(O/C\right)^{tg} - 1.3}{\left(O/H_2\right)^{tg} - 0.37} = \frac{0.7}{0.63} \quad (g)$$

Now equations (f) and (g) are simultaneous equations in $\left(O/C\right)^{tg}$ and $\left(O/H_2\right)^{tg}$ which can be solved to give the top gas composition as follows:

$$n_{CO}^{tg} = n_C^A \left[2 - \left(O/C\right)^{tg} \right] \quad (h)$$

$$n_{CO_2}^{tg} = n_C^A \left[\left(O/C\right)^{tg} - 1 \right] \quad (i)$$

$$n_{N_2}^{tg} = \frac{0.79}{0.21} \cdot \frac{1}{2} n_O^B \quad (j)$$

$$n_{H_2}^{tg} = Y n_{inj} \left[1 - \left(O/H_2\right)^{tg} \right] \quad (k)$$

$$n_{H_2O}^{tg} = Y n_{inj} \left[\left(O/H_2\right)^{tg} \right] \quad (l)$$

Now taking overall heat balance, we get,

$$\begin{aligned} D_{total} = & n_C^A \left\{ \left[2 - \left(O/C\right)^{tg} \right] \cdot H_{298}^f + \left\{ \left(O/C\right)^{tg} - 1 \right\} \cdot H_{CO_2}^f \right. \\ & + Y n_{inj} \left\{ \left[1 - \left(O/H_2\right)^{tg} \right] \cdot H_{H_2O}^f \right. \\ & + n_O^B \left\{ \frac{1}{2} \left[H_{O_2}^O \right] + \frac{0.79}{0.21} \frac{1}{2} \left[H_{N_2}^O \right] \right\} \\ & - n_C^A \left\{ \left[2 - \left(O/C\right)^{tg} \right] \left[H_{CO}^O - H_{CO}^{O_{298}} \right] + \left[\left(O/C\right)^{tg} - 1 \right] \left[H_{CO_2}^O - H_{CO_2}^{O_{298}} \right] \right\} \\ & + Y n_{inj} \left\{ \left[1 - \left(O/H_2\right)^{tg} \right] \left[H_{H_2}^O - H_{H_2}^{O_{298}} \right] \right. \\ & + \left. \left(O/H_2\right)^{tg} \left[H_{H_2O}^O - H_{H_2O}^{O_{298}} \right] \right\} \\ & - n_O^B \frac{1.79}{0.21} \cdot \frac{1}{2} \left[H_{N_2}^O \right] \end{aligned} \quad (m)$$

(If above equation reference temperature has been taken as

298K)

In equation (m), the only unknown is T_g (the temperature of the top gas). The values for heat of formation and enthalpy increments have been given in appendix I and II respectively. The modified model predicts the following information about the blast furnace -

- (1) Coke rate and air requirement of the blast furnace.
- (2) Top gas temperature and its composition.

APPENDIX IX

Typical coal composition of coals of different grades (on dry ash free basis) alongwith their calorific values [23]

Coal grade	% Volatile matter	% Fixed carbon	Gross calorific value (KJ/kg)
Meta-anthracite	1.3	98.7	31879
Anthracite	3.7	96.3	32177
Semi-anthracite	14.8	85.2	31641
Bituminous			
Low volatile	16.8	83.2	34950
Medium volatile	22.8	77.2	35365
High volatile A	36.7	63.3	33543
High volatile B	41.4	58.6	32872
High volatile C	40.0	60.0	31383
Sub-bituminous			
A	40.8	59.2	31676
B	44.0	56.0	30868
C	44.4	54.6	25863

APPENDIX X

Here the results obtained from the model for two-stage smelting reduction process have been presented in the tabular form (4.1 - 4.16). Tables 4.2, 4.4, 4.6, 4.8, 4.13 and 4.15 are valid for bituminous coal of composition :

% C = 86.4, % H = 4.9, % N = 1.6, % S = 0.6, % O = 3.6 and
% Ash = 2.9

whereas tables 4.3, 4.5, 4.7, 4.9, 4.14 and 4.16 are for sub-bituminous coal of composition :

% C = 64.2, % H = 4.4, % N = 1.2, % S = 0.4, % O = 16.6 and
% Ash = 13.2

Table 4.1 Thermal and chemical demand for various metallurgical operations at 0% and 100% metallization

<div style="text-align: center;"> SLAG RATE (KG/THM) COMPONENT </div>	350		450		550	
	0%	100%	0%	100%	0%	100%
HOT METAL	1.383*	1.383	1.383	1.383	1.383	1.383
SLAG	0.463	0.463	0.578	0.578	0.693	0.693
TOP GAS	0.663	0.663	0.663	0.663	0.663	0.663
LOSSES	0.335	0.335	0.335	0.335	0.335	0.335
ENDOTHERMIC HEAT REQUIRED IN RSF	2.983	6.262	3.834	7.113	4.690	7.969
ENDOTHERMIC HEAT REQUIRED IN MG	5.490	2.211	6.656	3.377	7.829	4.550
TOTAL DEMAND	11.317	11.317	13.449	13.449	15.593	15.593
REDUCTION GAS SENSIBLE HEAT	1.25	0.983	1.34	1.073	1.460	1.193

(* => ALL IN GJ/THM)

Table 4.2 Bituminous coal consumption at various degrees of metallization for different slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR	0	20	40	60	80	100
350	0	1733.92	1518.44	1302.96	1087.48	872.00	656.52
	10	1060.67	928.26	795.85	663.44	531.03	398.62
	20	747.76	653.59	559.42	465.25	371.08	276.91
450	0	1820.71	1605.23	1389.75	1174.26	958.78	743.30
	10	1145.02	1009.64	874.25	738.87	603.48	468.10
	20	835.53	738.83	642.14	545.44	448.75	352.05
550	0	1907.49	1692.01	1476.53	1261.05	1045.57	830.09
	10	1229.78	1088.54	947.30	806.06	664.82	523.58
	20	922.28	824.04	725.80	627.56	529.32	431.08

Table 4.3 Sub-bituminous coal consumption at various degrees of metallization for different slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR	0	20	40	60	80	100
350	0	2677.33	2296.36	1914.99	1533.62	1152.25	770.88
	10	2002.56	1726.26	1449.96	1173.66	897.36	621.06
	20	1689.45	1455.53	1221.61	987.69	753.77	519.85
450	0	2775.79	2387.30	1998.81	1610.33	1221.84	833.35
	10	2098.08	1817.52	1536.96	1256.40	975.84	695.28
	20	1786.98	1540.42	1293.86	1047.30	800.74	554.18
550	0	2874.31	2481.71	2089.11	1696.51	1303.91	911.31
	10	2192.21	1906.56	1620.91	1335.26	1049.61	763.96
	20	1881.11	1621.79	1362.47	1103.15	843.83	584.51

Table 4.4 O₂ requirements for bituminous coal consumption at various degrees of metallization for different slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR		0	20	40	60	80	100
350	0	C	2387.17	2084.84	1782.51	1480.18	1177.85	875.52
		P	0	0	0	0	0	0
	10	C	1433.90	1245.80	1057.70	869.60	681.50	493.40
		P	102.74	90.53	78.32	66.11	53.9	41.69
	20	C	997.76	864.5	731.24	597.98	464.72	331.46
		P	170.15	151.14	132.13	113.12	94.11	75.10
450	0	C	2524.95	2222.61	1920.26	1617.92	1315.58	1013.24
		P	0	0	0	0	0	0
	10	C	1575.66	1385.90	1196.13	1006.37	816.60	626.84
		P	123.43	108.80	94.17	79.53	64.90	50.27
	20	C	1140.85	1002.65	864.45	726.26	588.06	449.86
		P	179.96	158.63	137.29	115.96	94.62	73.29
550	0	C	2662.73	2360.37	2058.02	1755.66	1453.31	1150.95
		P	0	0	0	0	0	0
	10	C	1741.37	1550.12	1358.87	1167.62	976.37	785.12
		P	187.47	167.84	148.21	128.58	108.95	89.32
	20	C	1306.56	1160.24	1013.92	867.60	721.28	574.96
		P	236.23	212.54	188.85	165.16	141.47	117.78

(C => OXYGEN FOR COAL COMBUSTION; P => OXYGEN FOR POST-COMBUSTION)

Table 4.5 O₂ requirements for sub-bituminous coal consumption
at various degrees of metallization for different
slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR		0	20	40	60	80	100
350	0	C	2499.48	2131.28	1763.08	1394.88	1026.68	658.48
		P	0	0	0	0	0	0
	10	C	1528.48	1338.57	1148.66	958.75	768.84	578.93
		P	121.44	105.17	88.9	72.63	56.36	40.09
	20	C	1066.23	912.89	759.55	606.21	452.87	299.53
		P	189.63	171.81	153.99	136.17	118.35	100.53
450	0	C	2638.35	2263.21	1888.07	1512.92	1137.78	762.64
		P	0	0	0	0	0	0
	10	C	1674.64	1482.08	1289.52	1096.96	904.4	711.84
		P	158.76	139.46	120.16	100.86	81.56	62.26
	20	C	1223.42	1067.11	910.80	754.49	598.18	441.87
		P	215.30	192.69	170.08	147.47	124.86	102.25
550	0	C	2781.46	2389.87	1998.28	1606.69	1215.10	823.51
		P	0	0	0	0	0	0
	10	C	1826.76	1623.16	1419.56	1215.96	1015.36	808.76
		P	231.11	206.94	182.77	158.6	134.43	110.26
	20	C	1419.86	1258.28	1096.70	935.12	773.54	611.96
		P	287.47	257.42	227.37	197.32	167.27	137.22

(C => OXYGEN FOR COAL COMBUSTION; P => OXYGEN FOR POST-COMBUSTION)

Table 4.6 (CO + H₂) production when bituminous coal is combusted at various degrees of metallization for different slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR	0	20	40	60	80	100
350	0	3726.19	3493.30	2794.63	2328.84	1863.06	1397.28
	10	2023.54	1762.13	1500.72	1239.31	977.9	716.49
	20	1245.65	1075.54	905.43	735.32	565.21	395.1
450	0	3929.21	3463.43	2997.64	2531.86	2066.07	1600.29
	10	2221.77	1958.39	1695.01	1431.63	1168.25	904.87
	20	1439.72	1269.05	1098.37	927.70	757.02	586.35
550	0	4132.23	3666.45	3200.66	2734.88	2269.10	1803.31
	10	2414.00	2148.11	1882.22	1616.33	1350.44	1084.55
	20	1627.07	1455.62	1284.17	1112.72	941.27	769.82

Table 4.7 (CO + H₂) production when sub-bituminous coal is combusted at various degrees of metallization for different slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR	0	20	40	60	80	100
350	0	4482.16	3932.40	3382.64	2832.88	2283.12	1733.36
	10	2773.93	2405.41	2036.89	1668.37	1299.85	931.33
	20	1992.39	1732.58	1472.77	1212.96	953.15	693.34
450	0	4687.97	4132.39	3576.81	3021.23	2465.64	1910.06
	10	2974.41	2974.41	2231.91	1860.66	1489.41	1118.16
	20	2186.95	1921.62	1656.29	1390.96	1125.63	860.30
550	0	4893.6	4330.73	3767.86	3204.99	2642.12	2079.25
	10	3170.46	2795.17	2419.88	2044.59	1669.3	1294.01
	20	2374.14	2102.02	1829.9	1557.78	1285.66	1013.54

Table 4.8 Surplus reduction gas ($\text{CO} + \text{H}_2$) amount and calorific value when bituminous coal is combusted at various degrees of metallization for different slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR		0	20	40	60	80	100
350	0	A	3317.5	2690.21	2062.92	1435.63	808.34	181.05
		C	46.5	38.4	30.3	22.2	14.1	6.0
	10	A	1668.80	1242.67	816.54	390.41	0	0
		C	26.04	20.09	14.14	8.19	0	0
	20	A	910.34	622.19	334.04	0	0	0
		C	16.86	12.26	7.66	0	0	0
450	0	A	3520.52	2892.3	2264.08	1635.86	1007.64	379.08
		C	49.7	42.8	35.9	29.0	22.1	15.2
	10	A	1867.03	1433.55	1000.07	566.59	133.11	0
		C	28.10	23.8	19.4	15.1	10.7	0
	20	A	1104.41	776.94	449.47	122.0	0	0
		C	18.2	15.0	11.8	8.7	0	0
550	0	A	3723.54	3095.25	2466.96	1838.67	1210.38	582.10
		C	52.3	45.4	38.5	31.6	24.7	17.8
	10	A	2059.32	1608.19	1157.05	705.92	254.79	0
		C	30.1	25.8	21.5	17.2	12.9	0
	20	A	1291.76	929.03	566.31	203.59	0	0
		C	19.5	16.3	13.1	9.90	0	0

(A => AMOUNT ; C => CALORIFIC VALUE)

Table 4.9 Surplus reduction gas (CO + H₂) amount and calorific value when sub-bituminous coal is combusted at various degrees of metallization for different slag rates and post combustion ratios (case 1)

SLAG AMOUNT (KG/THM)	%M PCR		0	20	40	60	80	100
350	0	A	4073.47	3359.53	2645.59	1931.65	1217.71	503.77
		C	58.3	49.8	41.3	32.8	24.3	15.8
	10	A	2419.19	1867.87	1316.55	765.23	213.91	0
		C	35.23	28.6	21.97	15.34	8.71	0
	20	A	1657.08	1207.22	757.36	307.5	0	0
		C	25.72	21.02	16.32	11.62	0	0
450	0	A	4279.28	3561.19	2843.10	2125.02	1406.94	688.85
		C	59.40	51.30	43.30	35.20	27.20	19.10
	10	A	2619.73	2063.23	1506.74	950.25	393.76	0
		C	37.0	31.0	25.0	19.0	13.0	0
	20	A	1851.64	1395.04	938.44	481.84	0	0
		C	26.8	22.1	17.4	12.7	0	0
550	0	A	4484.91	3759.54	3034.16	2308.78	1583.14	858.04
		C	64.5	56.4	48.3	40.2	32.1	24.0
	10	A	2815.78	2255.25	1694.71	1134.18	573.65	0
		C	39.9	33.8	27.7	21.6	15.5	0
	20	A	2038.83	1575.43	1112.04	648.65	185.26	0
		C	27.2	22.5	17.8	13.1	8.4	0

(A => AMOUNT ; C => CALORIFIC VALUE)

Table 4.10 Top gas amount and its calorific value

%M PCR		0	20	40	60	80	100
0	A	278.16	389.48	500.30	611.10	721.91	832.73
	C	12.9	15.04	17.18	19.32	21.46	23.6
10	A	241.84	368.16	494.49	620.79	747.11	873.43
	C	12.6	14.9	17.2	19.5	21.80	24.10
20	A	228.64	359.06	489.49	619.68	748.24	880.78
	C	10.2	13.0	15.8	18.6	21.4	24.2

(A => AMOUNT ; C => CALORIFIC VALUE)

Table 4.11 Top gas composition for various degrees of metallization

% M	% CO	% CO2	%H2	% H2O	%N2
0	73.87	0.26	25.17	0.11	0.58
10	73.48	0.64	24.85	0.42	0.58
20	72.74	1.37	24.37	0.91	0.58
30	71.90	2.21	23.82	1.46	0.58
40	70.93	3.18	23.18	2.10	0.58
50	69.79	4.31	22.43	2.85	0.58
60	68.45	5.65	21.55	3.75	0.58
70	66.83	7.26	20.49	4.81	0.58
80	64.85	9.23	19.19	6.12	0.58
90	62.37	11.71	17.56	7.76	0.58
100	58.75	15.30	15.95	9.38	0.58

Table 4.12 Reduction gas composition for various PCRs

Bituminous

%PCR	% CO	%CO2	%H2	%H2O	%N2
0	74.13	0	25.28	0	0.58
10	66.63	7.40	22.80	2.53	0.58
20	59.26	14.80	20.26	5.06	0.58
30	51.83	22.20	17.74	7.60	0.58
40	44.41	29.61	15.22	10.15	0.58
50	37.0	37.0	12.70	12.70	0.58

Subbituminous

%PCR	% CO	%CO2	%H2	%H2O	%N2
0	61.0	0	38.53	0	0.47
10	54.9	6.1	34.68	3.85	0.47
20	48.8	12.2	30.83	7.70	0.47
30	42.7	18.3	26.98	11.55	0.47
40	36.6	24.4	23.13	15.40	0.47
50	30.5	30.5	19.26	19.26	0.47

**Table 4.13 Coal rate, O₂ requirements and (CO + H₂) production
for case 2 when bituminous coal is used**

SLAG AMOUNT KG/THM	% PCR	COAL RATE (KG/THM)	O2 REQUIREMENT (NM3/THM)		(CO + H2) PRODUCTION (NM3/THM)
350	0	1755.42	C	2432.37	3785.99
			P	0	
	10	1213.81	C	1702.18	2321.8
			P	138.78	
	20	924.17	C	1310.91	1554.51
			P	199.62	
450	0	1852.23	C	2575.00	3997.35
			P	0	
	10	1303.72	C	1844.77	2530.52
			P	140.58	
	20	1006.16	C	1448.63	1734.79
			P	216.84	
550	0	1949.04	C	2717.63	4208.71
			P	0	
	10	1396.41	C	1984.37	2735.14
			P	152.71	
	20	1084.16	C	1580.2	1936.45
			P	236.86	

(C=> OXYGEN FOR COAL COMBUSTION; P=> OXYGEN FOR POST-COMBUSTION)

**Table 4.14 Coal rate, O₂ requirements and (CO + H₂) production
for case 2 when sub-bituminous coal is used**

SLAG AMOUNT KG/THM	% PCR	COAL RATE (KG/THM)	O2 REQUIREMENT (NM3/THM)		(CO + H2) PRODUCTION (NM3/THM)
350	0	2711.41	C	2554.48	4557.17
			P	0	
	10	2149.93	C	1824.84	3087.17
			P	141.09	
	20	1846.37	C	1431.97	2295.91
			P	229.46	
450	0	2812.09	C	2697.16	4768.64
			P	0	
	10	2250.86	C	1964.96	3298.77
			P	143.63	
	20	1937.9	C	1566.78	2502.54
			P	234.74	
550	0	2913.58	C	2839.48	4979.46
			P	0	
	10	2350.7	C	2102.89	3509.06
			P	157.26	
	20	2029.19	C	1695.52	2697.78
			P	240.82	

(C=> OXYGEN FOR COAL COMBUSTION; P=> OXYGEN FOR POST-COMBUSTION)

Table 4.15 Materials balance when bituminous coal is used

Slag rate Materials	350*	450	550
CaCO3	231.25 *	297.32	363.40
Iron ore	1527 *	1629.00	1712
%Fe2O3	87.32	84.50	80.42
%SiO2	6.72	7.05	7.78
% MnO	1.31	3.23	6.13
%Al2O3	3.75	4.28	5.18
%S	0.68	0.703	0.782
%P2O5	0.219	0.206	0.196

Table 4.16 Materials balance when sub-bituminous coal is used

Slag rate Materials	350 *	450	550
CaCO3	231.25 *	297.32	363.40
Iron ore	1431.0 *	1577.0	1659.0
%Fe2O3	87.01	85.71	82.33
%SiO2	6.02	6.21	6.38
% MnO	4.23	4.83	5.19
%Al2O3	1.74	2.21	3.66
%S	0.88	0.91	1.11
%P2O5	0.117	0.129	0.133

(* => KG/THM)